Derivation of Analytic Solution and MOC Calculation Procedure for Double Heterogeneity Treatment

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Abstract

The Sanchez-Pomraning method to resolve the double heterogeneity problem in the MOC transport calculation is described in detail. This method is founded on the collision probability method concepts which involves the collision and escape probabilities, and formally derived by using the statistical treatment of the neutron balance equation along a path. The statistical approach bring the concept of the chord and segment length distributions in the formulation of the integral equation for the grain surface and matrix fluxes, which later turns into collision and escape probabilities. For the analytic solution, a boundary layer of a grain thickness, in which no grain is present, is assumed within each flat source region. The analytic solution of the coupled integral equation which involves the convolution integral is derived first by Laplace transform, but finally by substitution. This solution introduces an effective cross section which represents the homogenized mixture of the matrix and grain. With observation that the resulting analytic solution for the matrix is the same as the MOC solution for the homogenized medium, the equivalent source is constructed so that the MOC calculation can be performed for the homogenized mixture. The assumption of the boundary layer causes, however, a problem in the neutron conservation which should be corrected by renormalization. This method requires very little modifications to the existing MOC code to implement the double heterogeneity treatment. Starting from the very basic collision probability relation, the exhaustive derivation and explanation of the all the solution and terms needed to establish the MOC calculation sequence with the double heterogeneity treatment are provided for complete understanding of the reader who might not have sufficient background on this subject.

1. Introduction

This monograph is to give a detailed description of the Sanchez-Pomraning method[1] to resolve the double heterogeneity problem in the method of characteristics (MOC) calculation. The MOC calculation with a double heterogeneity treatment need to be performed in the DeCART whole core transport code for applications to the conditions involving grains of fuel or burnable absorber admixed with a matrix. First of all, the double heterogeneity here means the additional level of heterogeneity introduced by the presence of tiny grains which need to be homogenized for practical calculation. Once the region containing the grains is homogenized, there will only a single level of heterogeneity which includes all the other heterogeneous constituents. The most typical example of the double heterogeneity is the VHTR core consisting of fuel blocks into which triso fuel bearing compacts are placed. In the compact, the base material is graphite and triply coated fuel particles or grains of ~0.5 mm in diameter are admixed. Since it is exhaustive to trace each tiny fuel particles, there is a strong need for homogenizing the compact in a practical transport calculation. The homogenization requires, however, special considerations because the triso fuel particles are not tiny optically for the neutrons of certain energies and the neutron flux essentially varies largely across the triso-grain to cause a large difference in the reaction rate between the explicit and smeared triso representation. Therefore, a much more delicate treatment than the trivial volume-weighted homogenization is needed for the micro-heterogeneity treatment.

The double heterogeneity problem was addressed by several researchers, most noticeably by Sanchez. He first used only the collision probability method (CPM) to perform the transport calculation as well as to generate the solution kernel and homogenized parameters for the stochastic mixture of the matrix and grains[2]. Later he replaced the CPM for transport calculation with the method of characteristics[3] which would relieve the assumption of the isotropic angular flux needed in the CPM transport solution. His most recent work[1] was to improve the solution for the non-conservation problem resulting from the neglect of the first layer of grains right inside the boundary during the analytic solution process. The three papers of Sanchez will be followed here with sufficient details including proofs and explanations of the physical meanings of each term or treatment. This detailed explanation is needed because his papers are quite abstract in many aspects. He omitted explanations for seemingly obvious things although such things are not clear to most readers who first encounter those.

The problem to be solved here is a within-group transport problem in which the source is known at each region and also within each grain. The method for solving the transport problem involving double heterogeneity which is to be explained here consists of two parts: *a priori* generation of the solution kernel and the homogenization parameter, and then the subsequent MOC calculation to determine the average flux in the homogenized region and eventually the grain specific reaction rate. The solution kernel derived in terms of the CP concepts will be of prime importance in the determination of the homogenized cross sections and decomposing the grain specific reaction rate. Thus the most part of this monograph will be devoted to the derivation of the CP bearing solution which results from the analytic solution of so called the renewal equations (cf. Section 2.1) for a stochastic medium.

In the next section, the characteristics of the stochastic problem are presented first to provide a proper view of the problem that we are dealing with. The renewal equation which is the integral balance equation is then derived in this section. The second section is to explain the fundamentals of the CPM with essential relations and proofs which are needed in the subsequent derivation. The third section is to derive the CPM based solution method which results in a coupled linear system consisting of grain and matrix fluxes and collision probabilities. The fourth section is to derive the analytic solutions to the renewal equation for the cases with a homogeneous grain internal structure. The fitth section is to apply the CP bearing analytic solution kernel to the MOC calculation and then to resolve so called the boundary layer problem which results from the neglect of a thin layer of one grain thick during the derivation of the analytic solution. The last section is to incorporate the heterogeneous grains in the solution kernel.

2. Statistical Formulation of Neutron Balance Equation in Stochastic Medium

Suppose a neutron ray passing though a region in which grains of different types are dispersed in the base matrix. The configuration under consideration is depicted in Figure 1. The ray shown here can be a ray used in the MOC calculation and the base region is a flat source region(FSR). Here we denote the grain type by a positive integer, 1 through N (the number of grain types) and the matrix by material 0. For now, we don't consider the internal structure of the grain. It will be discussed in Sections 3.2 and 6.1. It is obvious from this figure that the neutron would encounter various arrangements of the grains during its travel because the occurrence of a certain configuration is stochastic. Under this circumstance, it is impractical to solve the neutron conservation equation deterministically and a statistical approach is needed. The statistical approach brings so called renewal equations which are detailed below. The term renewal comes from "renewal process" which is a special sequence of processes occurring repeatedly with a prescribed probability distribution function (PDF). A renewal process is distinguished from a Poisson process which is a time-continuous "Markov process" in that the PDF is a general one instead of an exponential PDF. Note that a Markov process is a process or event that occurs totally independently from the previous processes and it is governed by an exponential PDF.

2.1 Renewal Equations

In the statistical approach, it should be first noted that a position x, measured from the region entrance point for a particular ray, can be occupied by any one of the (N+1) materials. The probability of occupying a position with the i-th material would be it's volume fraction p_i. If we define the i-th material angular flux, $\varphi_i(x)$, the expected value of the flux would be simply:

$$\varphi(x) = \sum_{i=0}^{N} p_i \varphi_i(x) . \tag{1}$$

In order to determine $\varphi_i(x)$, we should consider various cases that the position x can be by the volume of material i. Suppose placing a ray segment within a grain type i as shown in Figure 2. The end point of the ray segment can be located either interior or at the boundary. In both cases, there could be various grain configurations which can have the end point either in the interior or on the boundary as shown by the example spheres in the figure. Similarly, the starting point of the ray segment can be placed either any point in the interior or on the boundary.
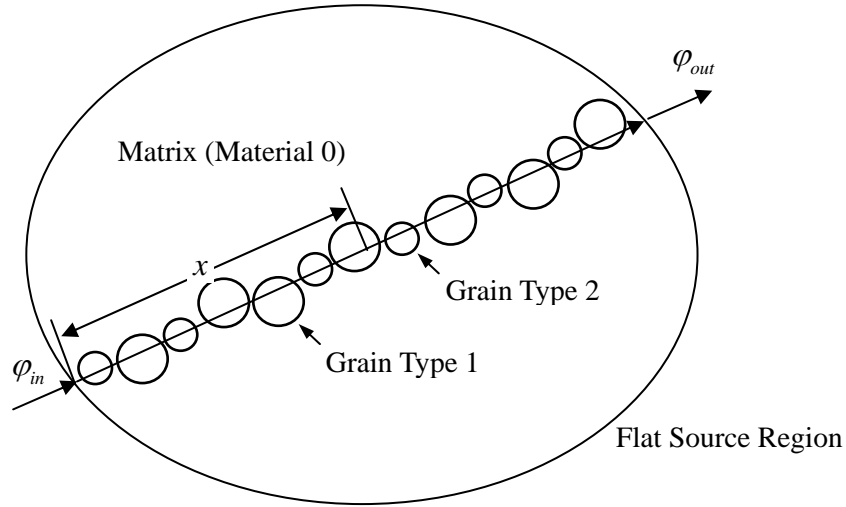
Figure 1. Ray passing through a stochastic medium

Now consider what contributions are there to affect $\varphi_i(x)$. There are only two contributions if $\varphi_i(x)$ is for grain flux. The first one is due to the surface source which originates from the incoming neutrons at the surface of the grain. The other one is due to the interior source which originates from fission and scattering within the grain. Let's denote the position of the source by y as the distance from x as shown in Figure 2. After traveling the distance y from the source, the neutrons would experience an exponential attenuation determined by the optical distance, $e^{-\Sigma_i y}$. This attenuation assumes that the entire path of length y is occupied by material i. But in the stochastic circumstance, there is a certain probability that the entire path is occupied by the material. Since there are two kinds of source, we need to consider two probabilities regarding the ray segment which are defined as follows:

$R_i(l)$ = probability that the distance from an interior point to a surface point is greater than l,

$g_i(l)dl$ = probability that the distance from an interior point to a surface point is greater than l but less than $l+dl$.

From the definition, the following relations are obvious:

$$R_i(l) = \int_l^{L_i} g_i(l')dl' = 1 - \int_0^l g_i(l')dl' \quad \text{or} \quad g_i(l) = -\frac{dR_i(l)}{dl} \tag{2}$$

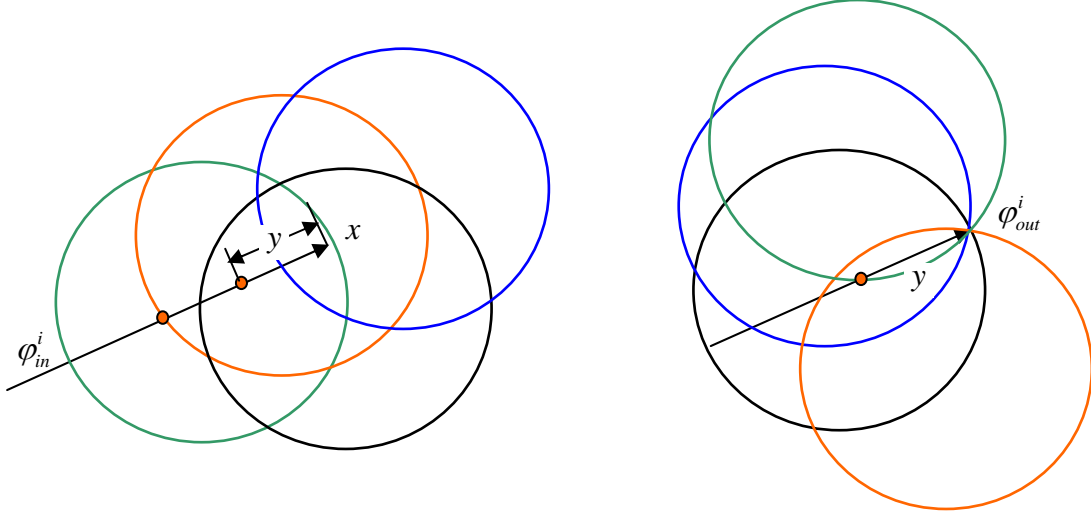with L_i being the maximum chord length of grain type *i*.

Figure 2. Various ray segment configurations for interior endpoint case (left) and surface endpoint case (right)

For a given interior source density, $S_i = \dfrac{1}{4\pi}\Sigma_s\phi + S_{ext}$ with S_{ext} specifying the external source consisting of the fission source and the in-scattering source, the intensity of the source located between *y* and *y+dy* would be $S_i dy$ (in fact we need to consider the cross sectional area δA of the ray since the source density is given per volume, but we do not use it explicitly because δA would appear in every term and can be cancelled out). On the other hand, the probability that the path between the source and the destination point (*x*) is occupied by material *i* is $R_i(y)$ since the surface point should be located beyond *y* from the source in order to have the path entirely occupied by material *i*. Thus the contribution from the infinitesimal source to $\varphi_i(x)$ is $S_i dy R_i(y)e^{-\Sigma_i y}$.

For the treatment of the surface source, we need to define first the incoming angular flux $\varphi_i^{in}(x)$ which is the expected incoming angular flux to material *i* at location *x*. For the incoming angular flux located away by *y* from *x*, $\varphi_i^{in}(x-y)$, the probability that the path from the infinitesimal surface source to an interior point *x* is occupied by material *i* is $g_i(y)dy$ which would yield the contribution from the surface source as $\varphi_i^{in}(x-y)g_i(y)dye^{-\Sigma_i y}$. In addition there can be an incoming source at the region boundary which specifies the boundary condition

at $x = 0$. This source at the origin is attenuated by $e^{-\Sigma_i x}$ and contributes to the flux with the material existence probability $R_i(x)$ for the travel distance of x. By combining the two sources which can occupy the position y and one from the source at the origin, we obtain the following integral equation for the material flux for an interior point:

$$\varphi_i(x) = \varphi_i(0) R_i(x) e^{-\Sigma_i x} + \int_0^x \left(S_i R_i(y) + \varphi_i^{in}(x-y) g_i(y) \right) e^{-\Sigma_i y} dy \; . \tag{3}$$

The incoming flux for the grain is related with the outgoing flux for the matrix and vice versa. If there is a transition a grain to the matrix, it can occur with any type of grains. Therefore, there is a certain probability for a grain to matrix transition for each grain type. Let t_i be the transition probability from grain type i to the matrix. Since once the transition to the matrix has to occur at a point, the transition must be with at least one of the grain types, the summation of the transition probabilities should sum up to 1.0, namely:

$$\sum_{i=1}^{N} t_i = 1 \; . \tag{4}$$

In terms of the transition probability and the grain outgoing angular flux, the incoming flux to matrix can be obtained as the following:

$$\varphi_0^{in}(x) = \sum_{i=1}^{N} t_j \varphi_j^{out}(x) \; . \tag{5}$$

The opposite, however, is very simple since the transition to a grain is possible only from the matrix. Namely, direct transition from a grain to another grain is not possible under the assumption that no grains contact each other. In this case, the incoming flux to any type of grain at location x is the same as the outgoing flux of the matrix, namely, $\varphi_i^{in}(x) = \varphi_0^{out}(x)$.

By replacing the incoming flux in Eq. (3) with the one of Eq. (5) which contains the outgoing fluxes, we have coupled equations in which the outgoing flux of the other materials are related with the internal flux of the material of interest. Since the outgoing flux which is the flux at the surface is also unknown, we need a separate balance equation for that.

For the flux at the surface, consider the following probabilities:

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$Q_i(l)$ = probability that the chord length is greater than l.

$f_i(l)dl$ = probability that the chord length is greater than l but less than $l+dl$.

Similarly to Eq. (2), we have:

$$Q_i(l) = \int_l^{L_i} f_i(l')dl' = 1 - \int_0^l f_i(l')dl' \quad \text{or} \quad f_i(l) = -\frac{dQ_i(l)}{dl} \tag{6}$$

With these probabilities, the balance equation for the outgoing flux reads

$$\varphi_i^{out}(x) = \varphi_i(0)Q_i(x)e^{-\Sigma_i x} + \int_0^x \left(S_i Q_i(y) + \varphi_i^{in}(x-y)f_i(y) \right)e^{-\Sigma_i y}dy \ . \tag{7}$$

The reason for using $Q_i(y)$ instead of $R_i(y)$ in the first term of the integrand is that the chord length should be at least y in order to have the distance from an interior point to the surface greater than y (cf. the right figure in Figure 2. All the cases other than the green one have the chord length greater than y). The use of the chord length distribution for the incoming source term is obvious because it is for surface to surface connection. Eqs. (3) and (7) constitute the renewal equations which are coupled through Eq. (5). Before deriving the analytic solutions to the renewal equations, considerations on several segment length distributions are made in the following.

2.2 Chord Length Distribution

Within a convex body, a segment can be defined by connecting any two points. The segment can be a chord if the connection is made between two surface points. As shown later, the distribution of the interior segment lengths which specifies $g(l)$ is related with the chord length distribution $f(l)$. First of all, let's first find an analytic expression for the chord length distribution for a sphere.

2.2.1 Case of Sphere

From Figure 3, it is obvious that the probability that the chord length is in between l and $l+dl$ would be the area ratio of the circular strip formed by $d\theta$ around θ to the entire area of the sphere. We can note first the following relation between the angle and the chord length:
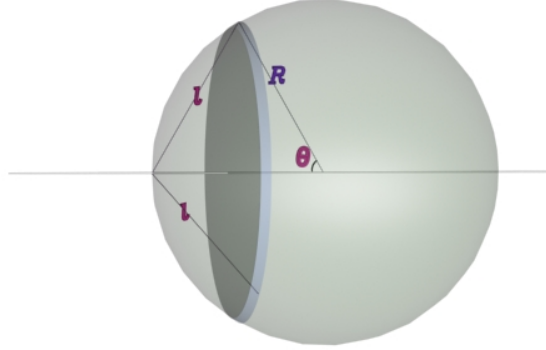
Figure 3. Chord length in a sphere

$$l = 2R \sin \frac{\theta}{2} . \tag{8}$$

and the radius of the strip is $R \sin \theta$ while the width is $R d\theta$. The probability that the end

point of the segment be located within the strip would then be:

$$p(\theta)d\theta = \frac{2\pi R \sin \theta \cdot R d\theta}{4\pi R^2} = \frac{\sin \theta}{2} d\theta . \tag{9}$$

This probability should be the same as the probability that the chord length is between l

and $l+dl$, namely:

$$f(l)dl = p(\theta)d\theta = \frac{\sin \theta}{2} d\theta . \tag{10}$$

From this and Eq. (8), we have

$$f(l) = \frac{\sin \theta}{2} \frac{d\theta}{dl} = \frac{\sin \theta}{2} \frac{1}{R \cos \frac{\theta}{2}} = \frac{\sin \frac{\theta}{2}}{R} = \frac{l}{2R^2} = \frac{2}{D}\left(\frac{l}{D}\right). \tag{11}$$

with the diameter *D* which is the maximum chord length. The probability that the chord length is greater than *l*, Q(*l*), is obtained by the integration of the above the probability distribution function (PDF):

$$Q(l) = \int_l^D f(l')dl' = 2\int_l^D \frac{l'}{D} d\frac{l'}{D} = 1 - \left(\frac{l}{D}\right)^2 . \tag{12}$$

The PDF for the chord length can also be used to determine the mean chord length:

$$\bar{l} = \int_0^D l'f(l')dl' = 2D\int_0^D \left(\frac{l'}{D}\right)^2 d\frac{l'}{D} = \frac{2}{3}D = \frac{4}{3}R = \frac{4V}{S} . \tag{13}$$

The probability that the distance from an interior point to the surface for a certain direction which is *R(l)* can be obtained based on Figure 4. The left sphere in the figure is the same one in the right. It is just shifted to the left by *l*. In this figure, we see that the probability that the distance to the surface be greater than *l* is merely the ratio of the volume of the common part of the two spheres to the total volume of the sphere. The volume of the common part is two time the volume of the shaded part which represents a cut of a sphere. The height of the cut is $R - \dfrac{l}{2}$.
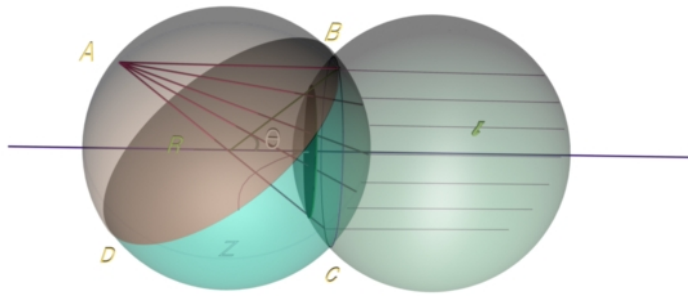

Figure 4. Distance from an interior point to surface

The volume of the cut is obtained by the integrating the volume of the disk located at *z* from the

top of the cut to the bottom. Noting that the radius of the disk is $\sqrt{R^2 - (R-z)^2}$, we have the volume of the cut as:

$$V_{cut} = \int_0^{R-\frac{l}{2}} \pi(R^2 - (R-z)^2)dz = \pi \int_0^{R-\frac{l}{2}} (2Rz - z^2)dz \qquad . \tag{14}$$
$$= \pi\left(R - \frac{l}{2}\right)^2 \left(R - \frac{1}{3}\left(R - \frac{l}{2}\right)\right) = \pi\left(R - \frac{l}{2}\right)^2 \left(\frac{2R}{3} + \frac{l}{6}\right)$$

The probability is now obtained as:

$$R(l) = \frac{2V_{cut}}{V_{sphere}} = \frac{2\pi\left(R - \frac{l}{2}\right)^2 \left(\frac{2R}{3} + \frac{l}{6}\right)}{\frac{4}{3}\pi R^3} = \left(1 - \frac{l}{2R}\right)^2 \left(1 + \frac{l}{4R}\right) \qquad . \tag{15}$$

The corresponding probability distribution function is now obtained by differentiation:

$$g(l) = -\frac{dR(l)}{dl} = -\frac{d}{dl}\left(1 - \frac{l}{2R}\right)^2\left(1 + \frac{l}{4R}\right) = \frac{1}{R}\left(1 - \frac{l}{2R}\right)\left(\left(1 + \frac{l}{4R}\right) - \frac{1}{4}\left(1 - \frac{l}{2R}\right)\right) . \tag{16}$$
$$= \frac{3}{4R}\left(1 - \left(\frac{l}{2R}\right)^2\right) = \frac{1 - \left(\frac{l}{2R}\right)^2}{\frac{4}{3}R} = \frac{1 - \left(\frac{l}{2R}\right)^2}{\bar{l}} = \frac{Q(l)}{\bar{l}}$$

As shown in the last of the above equation, the PDF for the internal segment distribution function can be obtained as the cumulative distribution function (CDF) divided by the mean chord length. This relation is further investigated below.

2.2.2 Relation between Segment PDF and Chord Length CDF

As can be seen in Figure 4, $g(l)dl$ would be the ratio of the volume of the disk located at the bottom of the cut (marked in green, the thickness of the disk is dl). The area of the disk is merely proportional to the surface area of the shell which spans from points B, C, and D (marked with the light green arc in Figure 4). Since the surface area of the shell is proportional to the CDF of the chord length as indicated by the green lines in Figure 4, the following relation holds:

$$g(l)dl = \alpha Q(l)dl$$

$$\text{(17)}$$

By imposing the normalization condition for the probability, we have

$$\alpha = \frac{1}{\int_0^L Q(l)dl} \cdot$$

$$\text{(18)}$$

Performing the integration of the denominator by parts, we have

$$\int_0^D Q(l')dl' = l'Q(l')\Big|_0^D - \int_0^D l'\frac{dQ(l')}{dl'}dl' = \int_0^D l'f(l')dl' = \bar{l} .$$

$$\text{(19)}$$

Note that the first term in the second expression above vanishes because *Q(L)=0*. Therefore, we have now the general relation between the PDF of the segment length and CDF of the chord length:

$$g(l) = \frac{Q(l)}{\bar{l}} .$$

$$\text{(20)}$$

Note that this is a generic relation holding for all the convex bodies.

3. Collision Probability Solution

The renewal equation can be solved analytically in terms of the various the collision probability concepts and terms. Before solving the renewal equations, we first derive various the collision probability relations and terms and then investigate the collision probability method (CPM) based solution of the double heterogeneity problem which involves construction of an equivalent homogenized problem with an approximation.

3.1 Basic Collision Probability Relations

Collision probability P_{ij} is defined as the probability for a neutron born isotropically and uniformly in volume j to have its first collision in volume i. Since we suppose only one neutron in V_j, the source density is $\dfrac{1}{V_j}$. For a unit isotropic source density at position $\vec{r}_j$, the flux at position $\vec{r}_i$ would be given as follows which reflects the geometrical spread and attenuation during the travel:

$$n(\vec{r}_j \to \vec{r}_i) = \frac{e^{-\rho(\vec{r}_i - \vec{r}_j)}}{4\pi R^2}. \tag{21}$$

where $\rho(\vec{r}_j - \vec{r}_i)$ is the optical distance between $\vec{r}_j$ and $\vec{r}_i$ that is determined by the macroscopic cross sections and the travel length at each interval of the line segment connecting $\vec{r}_j$ and $\vec{r}_i$. R is the distance between the two points. For collisions in V_i, the flux given by Eq. (21) should be multiplied by the total cross section Σ_i. With the source density of $\dfrac{1}{V_j}$, the first collision probability for V_j to V_i collision is then obtained as:

$$P_{ij} = \int_{V_i} \Sigma_i \int_{V_j} \frac{1}{V_j} n(\vec{r}_j \to \vec{r}_i) dV_j dV_i. \tag{22}$$

This brings the following reciprocity relation:

$$\frac{P_{ij}V_j}{\Sigma_i} = \int_{V_i}\int_{V_j} n(\vec{r}_j \to \vec{r}_i)dV_jdV_i = \frac{P_{ji}V_i}{\Sigma_j} \quad \text{or} \quad V_j\Sigma_jP_{ij} = V_i\Sigma_iP_{ji}. \qquad (23)$$

Now consider the escape probability E_i and the first-flight blackness γ_i. E_i is the probability for a neutron born in volume i to escape the volume without any collision while γ_i is the probability for a neutron entering an external surface uniformly with the isotropic angular distribution to have the first collision in volume i.

Suppose the volume configuration shown in Figure 5. The entire volume (V) is surrounded by a surface whose area is S and there is an internal volume V_i. Outside the volume there is a uniform and isotropic source density Q which occupies the infinitesimal strip having thickness δt. With these definitions, let's first obtain the escape probability. For one source neutron in V_i which would give the source density of $\frac{1}{V_i}$, E_i is obtained as:

$$E_i = \int_{V_i}\int_S \frac{1}{V_i}n(\vec{r}_j \to \vec{r}_i)dA_jdV_i . \qquad (24)$$

This is the survival probability of a neutron born in V_i passing through S.

The isotropic neutron source residing outside the external surface yields a *cosine* current distribution which means that the number of neutrons coming through any unit surface area has a cosine angular dependence because the entrance area to be seen by the neutron has the cosine dependence. For the cosine current, only $\frac{1}{4}$ of the source neutrons can pass through the surface due to the cosine dependence of the projected area. This can be easily seen by the following:

$$Q_{in} = \int_{2\pi}\int_0^{\frac{\pi}{2}} \frac{Q}{4\pi}\cos\theta\sin\theta d\theta d\alpha = \frac{Q}{2}\int_0^1 \mu d\mu = \frac{Q}{4} . \qquad (25)$$

Since the volume of the thin shell is $S\delta t$, the total number of neutrons passing through surface S whose area is A is $\frac{Q}{4}A\delta t$. Among these neutrons the following number of neutrons will have the first collision in V_i:

$$R_{col} = \int_{V_i} \int_{S_j} \Sigma_i Q \, n(\vec{r}_j \to \vec{r}_i) dA_j \delta t dV_i \, .$$ (26)

δt

S

$\vec{r}_i$ V_i V

dA

Q

$\vec{r}_j$
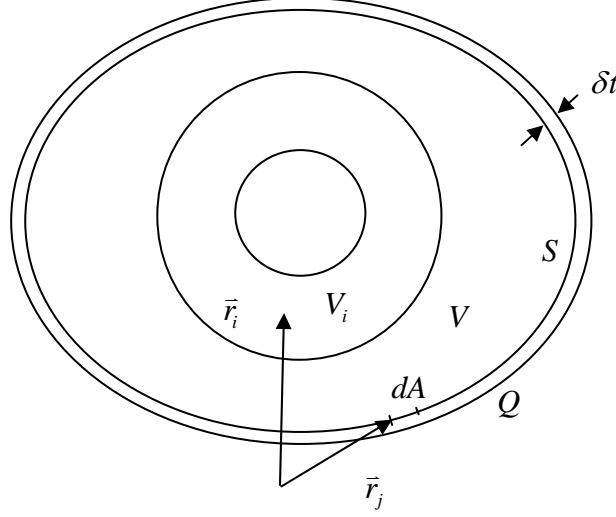
Figure 5. Escape probability vs. first-flight blackness calculation configuration

By definition the first flight blackness is obtained as:

$$\gamma_i = \frac{R_{col}}{Q_{in}} = \frac{\int_{V_i} \int_{S_j} \Sigma_i Q \, n(\vec{r}_j \to \vec{r}_i) dA_j \delta t dV_i}{\dfrac{Q}{4} A \delta t} = \frac{4\Sigma_i}{A} \int_{V_i} \int_{S} \, n(\vec{r}_j \to \vec{r}_i) dA_j dV_i \, .$$ (27)

From this and Eq. (24), we have

$$\gamma_i = \frac{4\Sigma_i}{A} V_i E_i \quad \text{or} \quad \gamma_i = \frac{4V}{A} \frac{V_i}{V} \Sigma_i E_i = \bar{l} p_i \Sigma_i E_i \, .$$ (28)

where $\bar{l} = \dfrac{4V}{A}$ is the mean chord length and p_i is the volume fraction of the interior volume.

Between the escape probability and the collision probabilities, we have the following obvious normalization conditions:

$$E_i + \sum_{j=1}^{N} P_{ji} = 1 \,, \tag{29}$$

$$T + \overline{l} \sum_{i=1}^{N} p_i \Sigma_i E_i = 1 \tag{30}$$

where N is the number of interior volumes within the external surface and T is the transmission probability for a neutron entering through the external surface with a cosine current distribution.

3.2 Collision Probability Balance Equations

In general there is an internal structure in a grain consisting of layers. By denoting the grain type by i and the layer by k, we can define various collision probabilities:

$P_{ik,jl}^{g}$ = probability for a source neutron originating from the l-th layer of the j-th grain type to have its first collision at the k-th layer of the i-th grain type,

$P_{ik,0}^{g}$ = probability for a source neutron originating from the matrix (material 0) to have its first collision at the k-th layer of the i-th grain type,

E_{ik}^{g} = probability for a source neutron originating from the k-th layer of the i-th grain type to escape through the grain boundary,

The superscript g in the above symbols means *grain* which signifies that the quantity is defined for a single grain rather than the group of all the grains of the same type. Representing the number of grains by n_i, parameters without the superscript is defined for the group of grains. For instance, $V_i = n_i V_i^{g}$ is the total volume of the grain type i which would determine the corresponding volume fraction by $p_i = \dfrac{V_i}{V}$. Similarly, $P_{ik,0} = n_i P_{ik,0}^{g}$ is the probability for the transfer from the matrix to any grain of type i.

Suppose that we are now interested in the average reaction rate in each type of grain as well as in the matrix within a region which contains the mixture of the matrix and grains as shown in Figure 1. The first approach we can take to determine those reactions rates is to use the balance equation to be formed in terms of the collision probabilities (CP) as in the following subsection.

Before deriving the balance equation, suppose that isotropic neutron source densities are given

in each layer and matrix as $S_{ik} = \dfrac{1}{4\pi}\Sigma_{s,ik}\phi_{ik} + S_{ext,ik}$ and $S_0 = \dfrac{1}{4\pi}\Sigma_{s,0}\phi_0 + S_{ext,0}$. The first term is for the within group scattering while the second is for all the other sources. Out of the grain internal sources, there will be neutrons leaking out to the matrix which can be represented as:

$$J_+ = \sum_i n_i \sum_k E_{ik}^g V_{ik}^g S_{ik} = \sum_{i,k} E_{ik}^g V_{ik} S_{ik} \;. \tag{31}$$

This can be regarded as the surface source to the matrix. Using this surface and volume source of the matrix, the balance equations for the matrix and each grain layer can be written as follows in terms of the total collision rates:

$$V_0 \Sigma_0 \phi_0 = P_{00}(V_0 S_0 + J_+) \;, \tag{32}$$

$$V_{ik}^g \Sigma_{ik} \phi_{ik} = P_{ik,0}^g (V_0 S_0 + J_+) + \sum_l P_{ik,il}^g V_{il}^g S_{il} \;. \tag{33}$$

where P_{00} is the matrix-to-matrix collision probability. The first term of Eq. (33) signifies that all the neutrons coming outside of a grain enters it only through the matrix while the second term indicates the grain internal source coming from other layers. This is possible under the assumption that there is no direct contact between grains, which is quite reasonable.

By using Eq. (31) and multiplying n_i to Eq. (33), we have

$$V_0 \Sigma_0 \phi_0 = P_{00} V_0 S_0 + \sum_{i,k} P_{0,ik} V_{ik} S_{ik} \;, \tag{34}$$

$$\begin{aligned}
V_{ik}\Sigma_{ik}\phi_{ik} &= P_{ik,0}(V_0 S_0 + \sum_{j,l} E_{jl}^g V_{jl} S_{jl}) + \sum_l P_{ik,il}^g V_{il} S_{il} \\
&= P_{ik,0} V_0 S_0 + \sum_{j,l} P_{ik,0} E_{jl}^g V_{jl} S_{jl} + \sum_{j,l} \delta_{i,j} P_{ik,jl}^g V_{jl} S_{jl} \\
&= P_{ik,0} V_0 S_0 + \sum_{j,l} P_{ik,jl} E_{jl}^g V_{jl} S_{jl}
\end{aligned} \tag{35}$$

where the layer-to-matrix collision probability is defined as

$$P_{0,ik} = P_{00}E_{ik}^g \tag{36}$$

and the layer to layer collision probability is defined as

$$P_{ik,jl} = P_{ik,0}E_{jl}^g + \delta_{i,j}P_{ik,jl}^g \tag{37}$$

with the Kronecker delta $\delta_{i,j}$. Note that from the reciprocity relation, Eq. (23), layer-to-matrix collision probability can be obtained from matrix-to-layer collision probability:

$$P_{ik,0} = \frac{V_{ik}\Sigma_{ik}}{V_0\Sigma_0}P_{0,ik} \tag{38}$$

Eqs. (34) and (35) constitutes a linear system which is coupled through the source containing the flux. The linear system can be solved once the coefficients consisting of $E_{ik}^g, P_{ik,il}^g$ and P_{00} are known. The escape probability and the layer to layer collision probability can be determined by a suitable collision probability calculation routine. The matrix-to-matrix collision probability or matrix self collision probability, P_{00}, however, can not be obtained as such. It requires a special consideration which is to be described in the next subsection.

3.3 Determination of Matrix Self Collision Probability

The matrix self collision probability can be obtained through suitable homogenization of the region containing the matrix and grains. Let's denote the boundary of the region by Γ and define the transmission probability for the region by T and the escape probabilities for the matrix and grains associated with the region boundary Γ as E_0 and E_{ik}, respectively. Then the escape probability through Γ is related with the grain escape probability as:

$$E_{ik} = E_0E_{ik}^g \tag{39}$$

It is related with the region transmission probability through the following condition:

$$1 = T + \gamma_0 + \sum_i n_i \sum_k \gamma_{ik} \qquad \qquad . \tag{40}$$

$$= T + \frac{4V_0}{A}\Sigma_0 E_0 + \sum_i n_i \sum_k \frac{4V_{ik}^g}{A}\Sigma_{ik} E_{ik}$$

$$= T + \frac{4V}{A}\frac{V_0}{V}\Sigma_0 E_0 + \sum_i \sum_k \frac{4V}{A}\frac{V_i}{V}\frac{V_{ik}}{V_i}\Sigma_{ik} E_{ik}^g E_0$$

$$= T + \bar{l}p_0 \Sigma_0 E_0 + \bar{l}\sum_i p_i \sum_k \frac{V_{ik}}{V_i}\Sigma_{ik} E_{ik}^g E_0$$

The first equality of the above equation states that the probability for a neutron either to react within anywhere in the region (matrix of grain) or transmit should be 1.0 and the second equality comes from Eq. (28). The last term is further simplified as:

$$\bar{l}\sum_i p_i \sum_k \frac{V_{ik}}{V_i}\Sigma_{ik} E_{ik}^g E_0 = \bar{l}\sum_i p_i \sum_k \frac{\frac{4V_{ik}^g}{A_i^g}}{\frac{4V_i^g}{A_i^g}}\Sigma_{ik} E_{ik}^g E_0 \tag{41}$$

$$= \bar{l}\sum_i \frac{p_i}{\bar{l}_i}\sum_k \frac{4V_{ik}^g}{A_i^g}\Sigma_{ik} E_{ik}^g E_0$$

$$= \bar{l}E_0 \sum_i \frac{p_i}{\bar{l}_i}\sum_k \gamma_{ik}^g$$

$$= \bar{l}E_0 \sum_i \frac{p_i}{\bar{l}_i}\left(1 - T_i^g\right)$$

Note that grain mean chord length, $\bar{l}_i = \frac{4V_{ik}^g}{A_i^g}\gamma_{ik}^g$, and the reciprocity relation, Eq. (28), are applied at the grain level for the grain first-flight blackness, γ_{ik}^g, which is the probability for a neutron entering the grain surface of a Type i grain to have its first collision within Layer k. The summation of the grain first-flight blackness over all the layers is of course unity minus the grain transmission probability. By dividing both sides of the above equation by $\bar{l}E_0$, we have the following relation between the grain escape probability and the grain transmission probability:

$$\sum_i p_i \sum_k \frac{V_{ik}}{V_i}\Sigma_{ik} E_{ik}^g = \frac{1}{V}\sum_{i,k} V_{ik}\Sigma_{ik} E_{ik}^g = \sum_i \frac{p_i}{\bar{l}_i}\left(1 - T_i^g\right). \tag{42}$$

By inserting Eq. (41) into Eq. (40), the transmission probability is obtained as:

$$T = 1 - p_0 E_0 \bar{l} \tilde{\Sigma} \tag{43}$$

where

$$\begin{aligned}
\tilde{\Sigma} &= \Sigma_0 + \frac{1}{p_0} \sum_i \frac{p_i}{\bar{l}_i} \left(1 - T_i^g\right) \\
&= \Sigma_0 + \frac{1}{V_0} \sum_{i,k} V_{ik} \Sigma_{ik} E_{ik}^g .
\end{aligned} \tag{44}$$

On the other hand, the conservation relation for outward neutrons originating from the region reads:

$$1 = P_{00} + \sum_{i,k} P_{ik,0} + E_0 . \tag{45}$$

By using Eqs. (38) and (44), Eq. (45) can be converted into:

$$\begin{aligned}
1 - E_0 &= P_{00} + \sum_{i,k} \frac{V_{ik} \Sigma_{ik}}{V_0 \Sigma_0} P_{0,ik} \\
&= P_{00} + \sum_{i,k} \frac{V_{ik} \Sigma_{ik}}{V_0 \Sigma_0} E_{ik}^g P_{00} \\
&= \frac{P_{00}}{\Sigma_0} \left(\Sigma_0 + \frac{1}{V_0} \sum_{i,k} V_{ik} \Sigma_{ik} E_{ik}^g \right) \\
&= \frac{P_{00}}{\Sigma_0} \tilde{\Sigma}
\end{aligned} \tag{46}$$

which in turn together with Eq. (43) gives:

$$\begin{aligned}
P_{00} &= \frac{\Sigma_0}{\tilde{\Sigma}} (1 - E_0) \\
&= \frac{\Sigma_0}{\tilde{\Sigma}} \left(1 - \frac{1}{p_0 \bar{l} \tilde{\Sigma}} (1 - T) \right) .
\end{aligned} \tag{47}$$

Thus the problem of fining the matrix-self-collision probability turns into finding the region transmission probability. Determination of the region transmission probability requires an homogenization of the matrix and grains because it can't be calculated for the stochastic medium.

The transmission probability can be determined in an alternative way by counting the number of collisions (C) within the region for the unity, uniform and isotropic source entering the region boundary surface, namely, $T = 1 - C$. Let the region be homogeneous with the cross section Σ_h and ϕ_{hom} be the average scalar flux within the region induced by the unit surface source. Then the number of total collisions within the region would be:

$$C_{\text{hom}} = V \Sigma_h \phi_{\text{hom}} (\Sigma_h)$$

(48)

Here $\phi_{\text{hom}}(\Sigma_h)$ indicates that the *average* flux is dependent on the homogeneous cross section. Note that there should be a flux gradient within the region despite the medium is homogeneous. On the contrary, for the heterogeneous region, denote the average scalar flux of the matrix induced by the unit surface neutron source be ϕ_{het} and assume that the angular flux distribution around a grain be isotropic such that the net current passing through the unit surface area is one-fourth of the scalar flux at the surface of grain type i, ϕ_i^s. The number of total collisions for the heterogeneous case is then

$$C_{het} = V_0 \Sigma_0 \phi_{het} + \sum_i n_i A_i^g \frac{1}{4} \phi_i^s (1 - T_i^g) .$$

(49)

By denoting the grain surface to the matrix flux ratio by $K_i = \dfrac{\phi_i^s}{\phi_{het}}$ which can also be regarded the self shielding ratio, the above equation is converted as:

$$C_{het} = V \left(p_0 \Sigma_0 + \sum_i K_i \frac{n_i V_i^g}{V} \frac{A_i^g}{4 V_i^g} (1 - T_i^g) \right) \phi_{het} = V \left(p_0 \Sigma_0 + \sum_i K_i \frac{p_i}{l_i} (1 - T_i^g) \right) \phi_{het} . \quad (50)$$

The homogenized cross section can be obtained by finding the suitable cross section which would give the same number of collisions of the homogeneous case, Eq. (48) as the heterogeneous collision number of Eq. (50). But this requires finding the heterogeneous flux and the self shielding ratio as well as the homogeneous flux which is not trivial.

It is possible, however, to find a first order accurate homogenized cross section considering the limiting case of the grains consisting of the matrix material. This case is in fact the homogeneous case. Anyhow, under this condition the grain interior collision due to the surface

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source is balanced as:

$$V_i^g \Sigma_0 \phi_{hom}(\Sigma_0) = \frac{1}{4} \phi_i^s(\Sigma_0) A_i^g \gamma_i^g(\Sigma_0) . \tag{51}$$

Note that Σ_0 within the parenthesis indicates that the corresponding quantities are calculated using the matrix cross section. By using the reciprocity relation, Eq. (28), Eq. (51) can be converted as the following which will give an approximated the self-shielding factor

$$\Sigma_0 \phi_{hom}(\Sigma_0) = \frac{A_i^g}{4V_i^g} \gamma_i^g(\Sigma_0) \phi_i^s(\Sigma_0) = \frac{\gamma_i^g(\Sigma_0)}{\overline{l}_i} \phi_i^s(\Sigma_0) = \Sigma_0 E_i^g(\Sigma_0) \phi_i^s(\Sigma_0) , \tag{52}$$

$$K_i(\Sigma) \sim \frac{\phi_i^s(\Sigma_0)}{\phi_{hom}(\Sigma_0)} = \frac{1}{E_i^g(\Sigma_0)} . \tag{53}$$

By inserting Eq. (53) into Eq. (50) and then by equating Eqs. (48) and (50), we have the homogenized cross section as:

$$\Sigma_h = p_0 \Sigma_0 + \sum_i \frac{p_i(1 - T_i^g)}{\overline{l}_i E_i^g(\Sigma_0)} . \tag{54}$$

Once this homogenized cross section is determined, the region transmission probability can be calculated for the homogeneous configuration and then the matrix self collision probability can be determined by Eq. (47). Alternatively, the region self collision probability for the homogenized medium, $P(\Sigma_h)$, can be calculated to determine P_{00} by using the reciprocity relations and conservation relations of Eqs. (28) through (30) as the following:

$$P_{00} = \frac{\Sigma_0}{\tilde{\Sigma}} \left(1 - \frac{\gamma(\Sigma_h)}{p_0 \overline{l} \tilde{\Sigma}} \right) = \frac{\Sigma_0}{\tilde{\Sigma}} \left(1 - \frac{\Sigma_h E(\Sigma_h)}{p_0 \tilde{\Sigma}} \right) = \frac{\Sigma_0}{\tilde{\Sigma}} \left(1 - \frac{\Sigma_h}{p_0 \tilde{\Sigma}} (1 - P(\Sigma_h)) \right) . \tag{55}$$

4. Analytic Solution of Renewal Equations

Among the input parameters needed to specify completely the coupled renewal equations given by Eqs. (3), (7), and (5), the segment or chord length distributions for the grains is obtained easily by Eq. (11) and other relations described in Section 2.2.2. But other parameters such as the transition probability and the matrix chord length distribution need further consideration which is to be given in the next subsection. After the parameters are specified, the solution of the renewal equation is derived in the second section.

4.1 Transition Probability and Matrix Chord Length Distribution

In order to determine the incoming current to the matrix at a point, $\varphi_0^{in}(x)$, it should be assumed that a transition from any one of the grain type to the matrix occurs at the point. Since there are several possibilities for such transition, the incoming current to the matrix should consist of the weighted average of outgoing currents out of all the grain types. The weighting factor is the transition probability t_i used in Eq. (5). The transition probability would depend on the volume fraction of the grain type and the mean chord length. We can imagine that as the mean chord length increases, the transition probability would decrease because there is more chance to stay within the grain, rather than transition to the matrix. On the contrary, if one grain type is more than the other grain types, the transition probability for the grain type would be larger. From this observation, let $t_i = c \dfrac{p_i}{\overline{l_i}}$ with a proportional constant c. If there ought to be a transition from any grain to the matrix, the summation of all the grain to matrix transition probability should be unity, namely:

$$\sum_{i=1}^{N} t_i = c \sum_{i=1}^{N} \frac{p_i}{\overline{l_i}} = 1 \;\; \rightarrow \;\; c = \frac{1}{\displaystyle\sum_{i=1}^{N} \frac{p_i}{\overline{l_i}}} \; . \tag{56}$$

If there is only one grain type, the mean chord length of the matrix can be easily obtained by supposing that the matrix portion of the track length is proportional to its volume fraction. Namely, $\overline{l_0} = p_0(\overline{l_0} + \overline{l_1})$ or $p_0 = \dfrac{\overline{l_0}}{\overline{l_0} + \overline{l_1}}$ which will give $\overline{l_0} = \dfrac{p_0 \overline{l_1}}{1 - p_0} = p_0 \dfrac{\overline{l_1}}{p_1}$. In case of multiple grain types, we can think that the average grain chord length is an weighted average of

each grain's mean chord length. We can use the transition probability as the weighting factor since it is proportional to the volume fraction and sums up to unity. Then the following relation holds (cf. Figure 6):

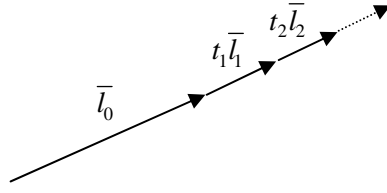$$p_0 = \frac{\overline{l}_0}{\overline{l}_0 + \sum_{i=1}^{N} t_i \overline{l}_i} \cdot \tag{57}$$

Figure 6. Constituents of an average ray

Since $t_i \overline{l}_i = c p_i$ and $\sum_{i=1}^{N} p_i = 1 - p_0$, the above equation can be converted to

$$p_0 = \frac{\overline{l}_0}{\overline{l}_0 + c(1 - p_0)} \rightarrow \overline{l}_0 = p_0 c \quad \text{or} \quad t_0 = c \frac{p_0}{\overline{l}_0} = 1 \,. \tag{58}$$

From Eq. (56), we now have the following relation which determines $\overline{l}_0$

$$\frac{p_0}{\overline{l}_0} = \sum_{i=1}^{N} \frac{p_i}{\overline{l}_i} \tag{59}$$

and

$$t_i = \frac{\overline{l}_0}{p_0} \frac{p_i}{\overline{l}_i} \,. \tag{60}$$

For the matrix chord length distribution, we can think of a binomial distribution with a large number of trials. Each event is to pickup a molecule of either matrix or grain material then to place it randomly on a line. If there is k successive occurrences of the grain material after n ($>k$) trial, the matrix chord length proportional to k is obtained. The sequence of the k matrix molecules does not matter so that it forms a binomial distribution. Since the probability of

placing a molecule in a specific position is very small, the binary distribution becomes a Poisson distribution which is represented by an exponential function ce^{-ax}. By imposing the normalization condition and the requirement of the mean chord length, the exponential distribution for the matrix chord length distribution is determined as:

$$f_0(l) = \frac{1}{\bar{l_0}} e^{-\frac{l}{\bar{l_0}}} . \tag{61}$$

The cumulative distribution function $Q_0(l)$ is obtained then by the integration

$$Q_0(l) = \int_0^\infty \frac{1}{\bar{l_0}} e^{-\frac{l'}{\bar{l_0}}} dl' = e^{-\frac{l}{\bar{l_0}}} . \tag{62}$$

Consequently, the PDF for the internal segment length, $g_0(l) = \dfrac{Q_0(l)}{\bar{l_0}}$ is the same as $f_0(l)$

and $R_0(l) = Q_0(l)$.

4.2 Solution of Renewal Equation with Boundary Layer Approximation

The first term of the renewal equation of Eq. (7) is the region incoming source contribution term which involves the cumulative chord length distribution function $Q_0(l)$. As shown above for the matrix, $Q_0(l)$ is an exponential function which can be combined with the exponential attenuation factor. But for spherical grains, it is a quadratic polynomial. It can be expected that the term containing the quadratic polynomial multiplied to the exponential function may not exist. The removal of the first term in the renewal equation is not a serious approximation. Since the size of the grain is very small (L) and $Q_i(x) = R_i(x) = 0$ for $x > L_i$, the following renewal equation for the grain which does not have the region incoming source term is valid except for very thin boundary layer of thickness L_i.

$$\varphi_i^{out}(x) = \int_0^{L_i} \left(S_i Q_i(y) + \varphi_i^{in}(x-y) f_i(y) \right) e^{-\Sigma_i y} dy \quad (x > L_i) . \tag{63}$$

Note that the upper limit of the integral is set to the maximum chord length since beyond it the probabilities are 0. For the matrix the renewal equation with the exponential chord length distribution becomes:

$$\varphi_0^{out}(x) = \varphi_0(0)e^{-\tilde{\Sigma}_0 x} + \int_0^x \left(S_0 + \frac{1}{l_0}\varphi_0^{in}(x-y) \right)e^{-\tilde{\Sigma}_0 y}dy \,.$$
(64)

where $\tilde{\Sigma}_0 = \Sigma_0 + \dfrac{1}{\bar{l}_0}$. These two equations are coupled through

$$\varphi_0^{in}(x) = \sum_i t_i \varphi_i^{out}(x) \,.$$
(65)

Before solving the system of the renewal equations, Eqs. (63) and (64), we first need to note that a convolution integral is involved. This suggests to use the Laplace transform technique which can treat conveniently the convolution integral.

4.2.1 Laplace Transform Solution

The Laplace transform of Eq. (64) gives

$$\Phi_0^{out}(s) = \frac{\varphi_0(0)}{s+\tilde{\Sigma}_0} + \frac{S_0}{s}\frac{1}{s+\tilde{\Sigma}_0} + \frac{1}{\bar{l}_0}\frac{1}{s+\tilde{\Sigma}_0}\sum_i t_i \Phi_i^{out}(s) \,.$$
(66)

where

$$\Phi_i^{out}(s) = L(\varphi_i^{out}(x)) = \int_0^\infty \varphi_i^{out}(x)e^{-sx}dx \,.$$
(67)

Note that the convolution theorem of Laplace transform was used to represent the Laplace equation of the convolution integral with the product of the two Laplace transforms. Before performing Laplace transform of Eq. (63), rewrite the following factor appearing in the first term using the relation (20):

$$\int_0^{L_i} Q_i(y)e^{-\Sigma_i y}dy = \bar{l}_i \int_0^{L_i} g_i(y)e^{-\Sigma_i y}dy = \bar{l}_i E_i^g \,.$$
(68)

Note that the integral of the second term is the definition of the escape probability because it is

the expected value of the non-attenuation probability. With this constant, the Laplace transform of the first term of Eq. (63) becomes:

$$L\left(\int_0^{L_i} S_i Q_i(y) e^{-\Sigma_i y} dy\right) = \frac{S_i \bar{l_i} E_i^g}{s} .$$

(69)

For the Laplace transform of the second term, let's first change the upper limit of the integral to x from L_i which do not have any impact since $f_i(y) = 0$ for $y > L_i$ and also $x > L_i$ for grains. Also consider the matrix outgoing current instead of the grain incoming current noting that $\varphi_i^{in}(x) = \varphi_0^{out}(x)$ because transition to a grain is possible only from matrix (no grain-to-grain transition). Then the Laplace transform is performed as follows with the change of the order of integration and also the integration variable:

$$\begin{aligned}
L\left(\int_0^x \varphi_0^{out}(x-y) f_i(y) e^{-\Sigma_i y} dy\right) &= \int_0^\infty \int_0^x \varphi_0^{out}(x-y) f_i(y) e^{-\Sigma_i y} dy \, e^{-sx} dx \\
&= \int_0^\infty \int_y^\infty \varphi_0^{out}(x-y) e^{-sx} dx f_i(y) e^{-\Sigma_i y} dy \\
&= \int_0^\infty \int_y^\infty \varphi_0^{out}(x-y) e^{-s(x-y)} dx f_i(y) e^{-(\Sigma_i+s) y} dy \\
&= \int_0^\infty \int_0^\infty \varphi_0^{out}(\tau) e^{-s\tau} d\tau f_i(y) e^{-(\Sigma_i+s) y} dy \\
&= \Phi_0^{out}(s) \int_0^\infty f_i(y) e^{-(\Sigma_i+s) y} dy
\end{aligned}$$

(70)

The last integral of the above equation can be replaced by a quantity which has a physical meaning. Suppose first $s = 0$. The integral becomes then the transmission probability, namely:

$$\int_0^\infty f_i(y) e^{-\Sigma_i y} dy = T_i^g .$$

(71)

because the integral is the expected value of the surface-to-surface non-attenuation probability for the given cross section of Σ_i. Noting from this physical significance, define

$$\int_0^\infty f_i(y) e^{-(\Sigma_i+s) y} dy = T_i^g(s) .$$

(72)

By using Eqs. (69), (70), and (72), the Laplace transform of Eq. (63) becomes now:

$$\Phi_i^{out}(s) = \frac{S_i \bar{l_i} E_i^g}{s} + T_i^g(s) \Phi_0^{out}(s) .$$

(73)

By inserting Eq. (73) into Eq. (66) and then multiplying $s + \tilde{\Sigma}_0$ to both sides, we have

$$(s + \tilde{\Sigma}_0)\Phi_0^{out}(s) = \varphi_0(0) + \frac{S_0}{s} + \frac{1}{\overline{l}_0}\sum_i t_i\left(\frac{S_i \overline{l}_i E_i^g}{s} + T_i^g(s)\Phi_0^{out}(s)\right). \tag{74}$$

which can be rearranged as follows with $\dfrac{t_i \overline{l}_i}{\overline{l}_0} = \dfrac{p_i}{p_0}$ coming from Eq. (60):

$$\left(s + \tilde{\Sigma}_0 - \frac{1}{\overline{l}_0}\sum_i t_i T_i^g(s)\right)\Phi_0^{out}(s) = \varphi_0(0) + \frac{1}{s}\left(S_0 + \frac{1}{\overline{l}_0}\sum_i t_i \overline{l}_i E_i^g S_i\right). \tag{75}$$

$$= \varphi_0(0) + \frac{1}{s}\left(S_0 + \frac{1}{p_0}\sum_i p_i E_i^g S_i\right)$$

Before solving the above equation for $\Phi_0^{out}(s)$, introduce an approximation to remove the *s*-dependence of the transmission probability which causes nonlinearity:

$$\Sigma = \tilde{\Sigma}_0 - \frac{1}{\overline{l}_0}\sum_i t_i T_i^g(s). \tag{76}$$

Then we have

$$\Phi_0^{out}(s) = \frac{1}{s + \Sigma}\varphi_0(0) + \frac{1}{s}\frac{1}{s + \Sigma}\left(S_0 + \frac{1}{p_0}\sum_i p_i E_i^g S_i\right). \tag{77}$$

The inverse Laplace transform gives:

$$\varphi_0^{out}(x) = \varphi_0(0)e^{-\Sigma x} + \int_0^x e^{-\Sigma x'}dx'\left(S_0 + \frac{1}{p_0}\sum_i p_i E_i^g S_i\right) \tag{78}$$

$$= \varphi_0(0)e^{-\Sigma x} + \left(S_0 + \frac{1}{p_0}\sum_i p_i E_i^g S_i\right)\frac{1}{\Sigma}\left(1 - e^{-\Sigma x}\right)$$

$$= \varphi_0(0)e^{-\Sigma x} + \tilde{\varphi}_{as}\left(1 - e^{-\Sigma x}\right)$$

where

$$\tilde{\varphi}_{as} = \frac{1}{\Sigma} \left(S_0 + \frac{1}{p_0} \sum_i p_i E_i^g S_i \right)$$ (79)

4.2.2 Solution by Substitution for Outgoing Flux

The above solution involves the approximation of Eq. (76) which is not valid in general. But is does suggest the solution form of Eq. (78). We take the solution form of Eq. (78) as is, but now regard the cross section unknown. This is one way of resolving the nonlinearity as shown below.

Let the solution for matrix be

$$\varphi_0^{out}(x) = \varphi_0(0)e^{-\Sigma x} + \varphi_{as}\left(1 - e^{-\Sigma x}\right)$$ (80)

which contains the attenuation of the region incoming source and asymptopic buildup term. By plugging Eq. (80) into Eq. (63) for $\varphi_i^{in}(x)$ yields

$$\varphi_i^{out}(x) = S_i \overline{l}_i E_i^g + \int_0^{L_i} \left(\varphi_0(0)e^{-\Sigma(x-y)} + \varphi_{as}(1 - e^{-\Sigma(x-y)}) \right) f_i(y)e^{-\Sigma_i y}dy$$
$$= S_i \overline{l}_i E_i^g + (\varphi_0(0) - \varphi_{as})e^{-\Sigma x}\int_0^{L_i} e^{-(\Sigma_i - \Sigma)y} f_i(y)dy + \varphi_{as}\int_0^{L_i} e^{-\Sigma_i y} f_i(y)dy$$. (81)

By defining the normal grain transmission probability and the reduced grain transmission probability which corresponds to reduced cross section $\Sigma_i - \Sigma$ as:

$$T_i^g = \int_0^{L_i} e^{-\Sigma_i y} f_i(y)dy$$
$$\hat{T}_i^g = \int_0^{L_i} e^{-(\Sigma_i - \Sigma)y} f_i(y)dy$$ (82)
$$\tilde{\varphi}_i^{out} = S_i \overline{l}_i E_i^g$$

Eq. (81) is represented in a simplified form:

$$\varphi_i^{out}(x) = \varphi_0(0)\hat{T}_i^g e^{-\Sigma x} + \varphi_{as}\left(T_i^g - \hat{T}_i^g e^{-\Sigma x}\right) + \tilde{\varphi}_i^{out}$$. (83)

By inserting Eqs. (83) into Eq. (64), we have

$$\varphi_0^{out}(x) = \varphi_0(0)e^{-\tilde{\Sigma}_0 x}$$

$$+ \int_0^x \left(S_0 + \frac{1}{\overline{l_0}} \sum_i t_i \left(\varphi_0(0)\hat{T}_i^g e^{-\Sigma(x-y)} + \varphi_{as}\left(T_i^g - \hat{T}_i^g e^{-\Sigma(x-y)}\right) + \tilde{\varphi}_i^{out} \right) \right) e^{-\tilde{\Sigma}_0 y} dy$$

$$= \varphi_0(0)e^{-\tilde{\Sigma}_0 x}$$

$$+ \int_0^x \left(S_0 + \frac{1}{\overline{l_0}} \sum_i t_i (\tilde{\varphi}_i^{out} + \varphi_{as} T_i^g) \right) e^{-\tilde{\Sigma}_0 y} dy$$

$$+ e^{-\Sigma x} \int_0^x \frac{1}{\overline{l_0}} \sum_i t_i \left((\varphi_0(0) - \varphi_{as})\hat{T}_i^g \right) e^{-(\tilde{\Sigma}_0 - \Sigma)y} dy$$

$$= \varphi_0(0)e^{-\tilde{\Sigma}_0 x}$$

$$+ \left(S_0 + \frac{1}{\overline{l_0}} \sum_i t_i (\tilde{\varphi}_i^{out} + \varphi_{as} T_i^g) \right) \frac{1}{\tilde{\Sigma}_0} \left(1 - e^{-\tilde{\Sigma}_0 x} \right) \tag{84}$$

$$+ \frac{1}{\overline{l_0}} \sum_i t_i \left((\varphi_0(0) - \varphi_{as})\hat{T}_i^g \right) \frac{1}{\tilde{\Sigma}_0 - \Sigma} \left(e^{-\Sigma x} - e^{-\tilde{\Sigma}_0 x} \right)$$

$$= \frac{1}{\tilde{\Sigma}_0} \left(S_0 + \frac{1}{\overline{l_0}} \sum_i t_i (\tilde{\varphi}_i^{out} + \varphi_{as} T_i^g) \right)$$

$$+ \frac{1}{\tilde{\Sigma}_0 - \Sigma} \frac{1}{\overline{l_0}} \sum_i t_i \hat{T}_i^g \left(\varphi_0(0) - \varphi_{as} \right) e^{-\Sigma x}$$

$$+ \left(\varphi_0(0) - \frac{1}{\tilde{\Sigma}_0} \left(S_0 + \frac{1}{\overline{l_0}} \sum_i t_i (\tilde{\varphi}_i^{out} + \varphi_{as} T_i^g) \right) \right.$$

$$\left. - \frac{1}{\tilde{\Sigma}_0 - \Sigma} \frac{1}{\overline{l_0}} \sum_i t_i \hat{T}_i^g \left(\varphi_0(0) - \varphi_{as} \right) \right) e^{-\tilde{\Sigma}_0 x}.$$

By imposing term by term equality between Eq. (84) with Eq. (80), we have the following identities:

$$\frac{1}{\tilde{\Sigma}_0} \left(S_0 + \frac{1}{\overline{l_0}} \sum_i t_i (\tilde{\varphi}_i^{out} + \varphi_{as} T_i^g) \right) = \varphi_{as}, \tag{85}$$

$$\frac{1}{\tilde{\Sigma}_0 - \Sigma} \frac{1}{\overline{l_0}} \sum_i t_i \hat{T}_i^g = 1 \tag{86}$$

With these two equations, the coefficient of $e^{-\tilde{\Sigma}_0 x}$ of Eq. (84) becomes 0 automatically so that the third term disappears.

Together with Eqs. (60) and (44), Eq. (85) gives

$$\varphi_{as} = \frac{S_0 + \frac{1}{\overline{l_0}}\sum_i t_i \tilde{\varphi}_i^{out}}{\tilde{\Sigma}_0 - \frac{1}{\overline{l_0}}\sum_i t_i T_i^g} = \frac{S_0 + \frac{1}{\overline{l_0}}\sum_i t_i \overline{l_i} E_i^g S_i}{\Sigma_0 + \frac{1}{\overline{l_0}} - \frac{1}{\overline{l_0}}\sum_i t_i T_i^g}$$

$$= \frac{S_0 + \frac{1}{p_0}\sum_i p_i E_i^g S_i}{\Sigma_0 + \frac{1}{p_0}\sum_i \frac{p_i}{\overline{l_i}}(1-T_i^g)} = \frac{1}{\tilde{\Sigma}}\left(S_0 + \frac{1}{p_0}\sum_i p_i E_i^g S_i\right)$$

(87)

Note that Eq. (79) from the approximate solution would be the same as the above one if $\Sigma = \tilde{\Sigma}$. Eq. (86), however, determines the exact value of Σ as the following:

$$\Sigma = \tilde{\Sigma}_0 - \frac{1}{\overline{l_0}}\sum_i t_i \hat{T}_i^g = \Sigma_0 + \frac{1}{\overline{l_0}}\left(1 - \sum_i t_i \hat{T}_i^g\right)$$

(88)

This is the new homogenized cross section which can only be determined iteratively because $\hat{T}_i^g$ itself is dependent on Σ.

4.2.3 Interior and Final Solutions

So far the solution for the outgoing angular flux was obtained. In order to solve for the interior angular flux which is needed to determine the reaction rates, first of all we note that there is no distinction between the internal and outgoing flux for the matrix which is the dispersed medium, namely, $\varphi_0(x) = \varphi_0^{out}(x)$. Therefore we need to solve only the renewal equation for the grain interior flux which reads as follows with $\varphi_i^{in}(x) = \varphi_0^{out}(x)$:

$$\varphi_i(x) = \int_0^{L_i}\left(S_i R_i(y) + \varphi_0^{out}(x-y)g_i(y)\right)e^{-\Sigma_i y}dy \quad (x > L_i).$$

(89)

Note that the segment distribution probabilities are used above instead of the chord length distribution functions. The first term in the integral can be represented by the self collision probability by using Eqs. (2) and (68) as follows:

$$\int_0^{L_i} S_i R_i(y) e^{-\Sigma_i y} dy = \frac{S_i}{\Sigma_i} \left(-R_i(y) e^{-\Sigma_i y} \Big|_0^{L_i} - \int_0^{L_i} g_i(y) e^{-\Sigma_i y} dy \right) \tag{90}$$
$$= \frac{S_i}{\Sigma_i} (1 - E_i^g)$$
$$= \frac{S_i}{\Sigma_i} P_{ii}^g$$

where P_{ii}^g is the grain self-collision probability. By inserting the solution for the matrix, Eq. (83), into Eq. (89), the following solution is obtained:

$$\varphi_i(x) = \frac{S_i}{\Sigma_i} P_{ii}^g + \int_0^{L_i} \left(\varphi_0(0) e^{-\Sigma(x-y)} + \varphi_{as}(1 - e^{-\Sigma(x-y)}) \right) g_i(y) e^{-\Sigma_i y} dy \tag{91}$$
$$= \frac{S_i}{\Sigma_i} P_{ii}^g + \int_0^{L_i} \left((\varphi_0(0) - \varphi_{as}) e^{-\Sigma(x-y)} + \varphi_{as} \right) g_i(y) e^{-\Sigma_i y} dy$$
$$= \frac{S_i}{\Sigma_i} P_{ii}^g + (\varphi_0(0) - \varphi_{as}) e^{-\Sigma x} \int_0^{L_i} g_i(y) e^{-(\Sigma_i - \Sigma)y} dy + \varphi_{as} \int_0^{L_i} g_i(y) e^{-\Sigma_i y} dy$$
$$= \frac{S_i}{\Sigma_i} P_{ii}^g + (\varphi_0(0) - \varphi_{as}) e^{-\Sigma x} \hat{E}_i^g + \varphi_{as} E_i^g$$
$$= \varphi_0(0) \hat{E}_i^g e^{-\Sigma x} + \varphi_{as} (E_i^g - \hat{E}_i^g e^{-\Sigma x}) + \tilde{\varphi}_i \ .$$

where the reduced grain escape probability is defined as:

$$\hat{E}_i^g = \int_0^{L_i} g_i(y) e^{-(\Sigma_i - \Sigma)y} dy \tag{92}$$

and

$$\tilde{\varphi}_i = S_i \frac{P_{ii}^g}{\Sigma_i} \ . \tag{93}$$

Finally, the flux at any point is obtained as the weighted average of the matrix and all grain fluxes:

$$\varphi(x) = p_0 \varphi_0(x) + \sum_{i=1}^N p_i \varphi_i(x) \tag{94}$$
$$= \varphi_{as}(p_0 + \sum_{i=1}^N p_i E_i^g) + (\varphi_0(0) - \varphi_{as})(p_0 + \sum_{i=1}^N p_i \hat{E}_i^g) e^{-\Sigma x} + \sum_{i=1}^N p_i \tilde{\varphi}_i \ .$$

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5. Implementation of DH Analytic Solution in MOC Calculation

The method of characteristics (MOC) calculation is to trace the change in the ray intensity along the line of ray which is called the characteristic line since it represents the line of motion of the neutron. For the ray tracing, the problem domain and angular space need to be discretized. In the spatial discretization, small regions are defined which is called the flat source region (FSR) because the source as well as the cross sections are considered constant. In the stochastic medium, the physical flat source region would contain grains and the matrix. Thus the analytic solution obtained for the stochastic medium can apply. In the following, the basic solutions of the MOC are described first and the stochastic solution is combined with the MOC solution to give the solution for the grains as well as for the matrix within a flat source region. Considerations of the consequence of the boundary layer problem which was introduced to be able to obtain the analytic solution in the previous section will also be considered.

5.1 Basic MOC Solutions

Suppose a FSR in which the incoming intensity of a certain ray is specified. The balance equation along the ray is simple as:

$$\frac{d\varphi}{dx} = -\Sigma \varphi(x) + S \quad , \quad \varphi(0) = \varphi_{in} \tag{95}$$

whose analytic solution is

$$\varphi(x) = \varphi_{in} e^{-\Sigma x} + \frac{S}{\Sigma}\left(1 - e^{-\Sigma x}\right). \tag{96}$$

At the exit of the FSR for the ray which is away by L from the entrance point, the outgoing angular flux is obtained as

$$\varphi_{out} = \varphi_{in}(1 - \beta) + \frac{S}{\Sigma}\beta \tag{97}$$

where

$$\beta = 1 - e^{-\Sigma L} \tag{98}$$

which approaches to 1.0 as L increases. The difference between the outgoing and incoming angular fluxes is then:

$$\varphi_D = \varphi_{out} - \varphi_{in} = \beta\left(\frac{S}{\Sigma} - \varphi_{in}\right). \tag{99}$$

The average of $\varphi(x)$ along the path of L is

$$\bar{\varphi} = \frac{\varphi_{in} - \dfrac{S}{\Sigma}}{\Sigma L}\beta + \frac{S}{\Sigma} = \frac{S}{\Sigma} + \frac{\varphi_D}{\Sigma L}. \tag{100}$$

5.2 Incorporation of DH Analytic Solution into MOC Solution

If the FSR is a stochastic medium, the outgoing flux of the FSR would be the matrix outgoing flux which is given by Eq. (80). This is in the same form as the MOC solution of Eq. (96). By the comparison of Eqs. (80) and (96), we can see that the cross section to be used should be the effective cross section Σ defined by Eq. (88) and the effective source is should be

$$S = \Sigma\varphi_{as} = \frac{\Sigma}{\tilde{\Sigma}}\left(S_0 + \frac{1}{p_0}\sum_i p_i E_i^g S_i\right) \tag{101}$$

with the following newly defined cross sections which are obtained from the second line of the above equation by using Eqs. (56) and (60):

$$\tilde{\Sigma} = \Sigma_0 + \frac{1}{\bar{l}_0}\sum_{i=1}^N t_i\left(1 - T_i^g\right), \tag{102}$$

$$\Sigma = \Sigma_0 + \frac{1}{\bar{l}_0}\sum_i t_i(1 - \hat{T}_i^g). \tag{103}$$

Since the definition of Σ is implicit in that $\hat{T}_i^g$ is the transmission probability of Type i grain obtained when the grain cross section is diminished by Σ from Σ_i, the calculation of Σ should be done iteratively. Once the effective cross section is determined and the effective source which consists of the sources in the grain and in the matrix, the outgoing flux of the

region can be determined by Eq. (97) and also the average angular flux in the matrix by Eq. (100). The ray tracing can continue through the next region by using the outgoing current of Eq. (97) as the next incoming current.

During the ray tracing, the average angular flux in the matrix is updated by

$$\bar{\varphi}_0 = \frac{\varphi_{in} - \dfrac{S}{\Sigma}}{\Sigma L} \beta + \frac{S}{\Sigma} \tag{104}$$

whereas the average angular flux in the grain can be obtained from Eq. (91) which gives together with Eqs. (100) and (93):

$$\begin{aligned}
\bar{\varphi}_i &= \frac{\varphi_0(0) - \varphi_{as}}{\Sigma L} \hat{E}_i^g \beta + \varphi_{as} E_i^g + \tilde{\varphi}_i \\
&= \left(\bar{\varphi}_0 - \frac{S}{\Sigma} \right) \hat{E}_i^g + \varphi_{as} E_i^g + \tilde{\varphi}_i \\
&= \bar{\varphi}_0 \hat{E}_i^g + \varphi_{as} (E_i^g - \hat{E}_i^g) + P_{ii}^g \frac{S_i}{\Sigma_i} \ .
\end{aligned} \tag{105}$$

The grain average angular flux should be summed up to form the scalar flux. The scalar flux of the grain will then determine the source S_i by the multiplication of fission and scattering cross sections.

5.3 Resolution of Non-Conservative Formulation

It was assumed in the derivation of the analytic solution of the renewal equation that the region incoming current does not affect the grain flux by limiting the validity of Eq. (63) for $x > L_i$, But the solution given by Eq. (96) assumes the validity of the equation over the whole track length. This is so called the boundary layer problem which appears as the violation of the basic conservation relation. It can be shown by examining the balance between the total production and leakage over the track. By using the renewal solutions for the matrix and grains, Eqs. (80) and (91), the net production along the track is obtained:

$$R_{prod} = \int_0^L \left(p_0(S_0 - \Sigma_0\varphi_0(x)) + \sum_{i=1}^N p_i(S_i - \Sigma_i\varphi_i(x)) \right) dx \tag{106}$$

$$= p_0 \int_0^L \left(S_0 - (\Sigma_0(\varphi_0(0)e^{-\Sigma x} + \varphi_{as}(1-e^{-\Sigma x}))) \right) dx$$

$$+ \sum_{i=1}^N p_i \int_0^L \left(S_i - \Sigma_i \left(\hat{E}_i^g \varphi_0(0)e^{-\Sigma x} + \varphi_{as}(E_i^g - \hat{E}_i^g e^{-\Sigma x}) + \frac{P_{ii}^g}{\Sigma_i} S_i \right) \right) dx$$

$$= p_0 \left((S_0 - \Sigma_0\varphi_{as})L - \Sigma_0(\varphi_{in} - \varphi_{as})\frac{\beta}{\Sigma} \right)$$

$$+ \sum_{i=1}^N p_i \left((S_i - \Sigma_i\varphi_{as})E_i^g L - \Sigma_i\hat{E}_i^g(\varphi_{in} - \varphi_{as})\frac{\beta}{\Sigma} \right)$$

$$= L \left(p_0 S_0 + \sum_i p_i S_i E_i^g - \varphi_{as}(p_0\Sigma_0 + \sum_i p_i\Sigma_i E_i^g) \right)$$

$$+ (\varphi_{as} - \varphi_{in})\frac{\beta}{\Sigma} \left(p_0\Sigma_0 + \sum_{i=1}^N p_i\Sigma_i\hat{E}_i^g \right)$$

$$= (\varphi_{as} - \varphi_{in})\beta\frac{\hat{\Sigma}}{\Sigma}$$

where

$$\hat{\Sigma} = p_0\Sigma_0 + \sum_i p_i\Sigma_i\hat{E}_i^g . \tag{107}$$

and the term containing L above disappears due to the asymptotic flux given by Eq. (87) and the second definition of $\tilde{\Sigma}$ given by Eq. (44).

On the other hand, the leakage obtained by the MOC solution is given by Eq. (99), namely with $\frac{S}{\Sigma} = \varphi_{as}$ of Eq. (101):

$$\varphi_{out} - \varphi_{in} = \beta(\varphi_{as} - \varphi_{in}) . \tag{108}$$

The conservation of neutrons requires that the net production should be the same and the leakage which in other word requires the equality of Eqs. (106) and (108). The equality does not hold since $\hat{\Sigma} \neq \Sigma$. Therefore in order to force conservation it is necessary to adjust the outgoing current of the MOC solution such that it matches with that of Eq.(106). This can be done conveniently by using $\hat{\beta} = r\beta$ instead of β in Eq. (108), where $r = \frac{\hat{\Sigma}}{\Sigma}$ is the renormalization factor, only when obtaining the outgoing current. For the calculation of the

average angular flux in the matrix and grain, the regular value of β which is based on Σ should be used. This guarantees the net production term which can also be represented as

$L\left(p_0(S_0 + \Sigma_0\overline{\varphi}_0) + \sum_i p_i(S_i - \Sigma_i\overline{\varphi}_i) \right)$ instead of the one given in Eq. (106) be the same as the

adjusted leakage:

$$\varphi_{out} - \varphi_{in} = \hat{\beta}\left(\varphi_{as} - \varphi_{in}\right) \tag{109}$$

6. Treatment of Heterogeneous Grains

In the derivation of the analytic solution in Section 4, the internal structure of the grain was not considered. With the homogeneous grains, the knowledge of chord length distribution was enough to the construction and solution of the renewal equation. For the heterogeneous grains, however, which have the internal structures consisting of layers, the cross sections and sources depend on the relative position (or local position) within the material. In this case, the probability for each possible trajectory to pass through the material should be considered. This section refines the solution of the renewal equation considering the internal structures.

6.1 Trajectory Probability

We observe that a trajectory (or chord) is uniquely specified by a relative point $\mathbf{r}$ and a relative direction $\mathbf{\Omega}$ as shown the following figure.
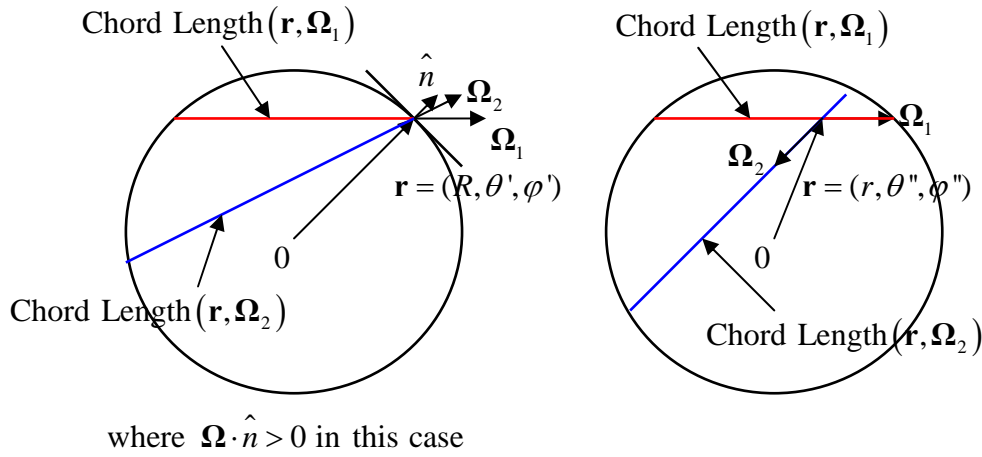

where $\mathbf{\Omega} \cdot \hat{n} > 0$ in this case

Figure 7. Trajectories specified by its exiting point $\mathbf{r}$ and its exiting direction $\mathbf{\Omega}$ (left) and an interior point $\mathbf{r}$ and a direction $\mathbf{\Omega}$ (right)

We consider two probabilities defined below:

$$f_i(\mathbf{r},\mathbf{\Omega})\left|\mathbf{\Omega}\cdot\hat{n}\right|d\mathbf{\Omega}dA = \text{probability that a phase point be around } (\mathbf{r},\mathbf{\Omega}) \text{ where } \mathbf{r}$$

is a point on the surface Γ_i^g of the grain and $\mathbf{\Omega}$ is an exiting direction in $(2\pi)_{out}$ at the point in $[\mathbf{\Omega},\mathbf{\Omega}+d\mathbf{\Omega}]$ and the position is within the surface element dA about $\mathbf{r}$,

$g_i(\mathbf{r},\mathbf{\Omega})d\mathbf{\Omega}dV$ = probability that a phase point be around $(\mathbf{r},\mathbf{\Omega})$ where $\mathbf{r}$ is a point within the volume V_i^g of the grain and $\mathbf{\Omega}$ is a direction in (4π) at the point in $[\mathbf{\Omega},\mathbf{\Omega}+d\mathbf{\Omega}]$ and position within the volume element dV about $\mathbf{r}$

The probability density functions $f_i(\mathbf{r},\mathbf{\Omega})$ and $g_i(\mathbf{r},\mathbf{\Omega})$ may depend on the specific ray and on the position x along the ray, but here we consider only homogeneous and isotropic statistics for which they depend only on $\mathbf{r}$ and $\mathbf{\Omega}$. The PDFs satisfy the normalization condition:

$$\int_{\Gamma_i^g}\int_{(2\pi)_{out}} f_i(\mathbf{r},\mathbf{\Omega})\left|\mathbf{\Omega}\cdot\hat{n}\right|d\mathbf{\Omega}dA = 1, \tag{110}$$

$$\int_{V_i^g}\int_{4\pi} g_i(\mathbf{r},\mathbf{\Omega})d\mathbf{\Omega}d\mathbf{r} = 1. \tag{111}$$

For a sphere, we can find $f_i(\mathbf{r},\mathbf{\Omega})$ in terms of the local spherical coordinate formed by taking the outward normal vector as the polar axis. Let the angle between the outward normal vector at $\mathbf{r}$ and $\mathbf{\Omega}$ be $\mathbf{\Omega}_n$. The $f_i(\mathbf{r},\mathbf{\Omega}_n)$ should then be constant for $0 < \theta_n < \dfrac{\pi}{2}$. In order to determine the constant, perform the following integration by changing the integration variable:

$$\int_{\Gamma_i^g}\int_{(2\pi)_{out}}\left|\mathbf{\Omega}\cdot\hat{n}\right|d\mathbf{\Omega}dA = \int_{\Gamma_i^g}\int_{(2\pi)_{out}}\cos\theta_n d\mathbf{\Omega}dA = \int_{\Gamma_i^g}\int_0^{\frac{\pi}{2}}\cos\theta_n 2\pi\sin\theta_n d\theta_n dA. \tag{112}$$

$$= 2\pi\int_{\Gamma_i^g}\int_0^1 \mu d\mu dA = 2\pi\int_{\Gamma_i^g}\frac{1}{2}dA = \pi A_i^g$$

From this and the normalization condition of (110), it is clear for a sphere that

$$f_i(\mathbf{r},\mathbf{\Omega}_n) = \begin{cases} \dfrac{1}{\pi A_i^g}, \text{ for outward directions} . \\ 0 \quad\text{ , for inward directions} \end{cases} \tag{113}$$

From this it can be inferred that in order to perform the integration over the angle only for the outward angle, the angular distribution function $\pi A_i^g f_i(\mathbf{r},\mathbf{\Omega}_n)$ must be used in the integrand which will give the value of unity only for the outward angle.

6.2 Interface Flux

As for the homogeneous grain, there are two contributions in the heterogeneous grain if $\varphi_i^{out}(x)$ is for grain flux. The first one is due to the surface source which originates from the incoming neutrons at the surface of the grain. The other one is due to the interior source consisting of the fission and scattering within the grain. Let's denote the position of the first source by $x - l(\mathbf{r}, \mathbf{\Omega})$ in the absolute coordinate and the second source by $\mathbf{r} - z\mathbf{\Omega}$ in relative coordinate as shown below.
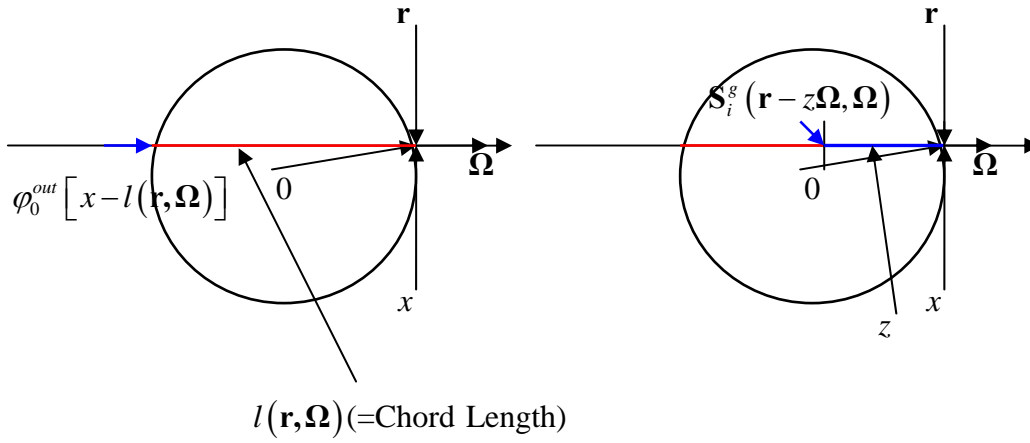

Figure 8. Two sources contributing to $\varphi^{out}(x)$

After traveling the distance $l(\mathbf{r}, \mathbf{\Omega})$ from the first source (incoming source), the neutrons in a certain $(\mathbf{r}, \mathbf{\Omega})$ would experience an exponential attenuation determined by the optical distance, $e^{-\tau_i(\mathbf{r}, \mathbf{\Omega}, l(\mathbf{r}, \mathbf{\Omega}))}$, where $\tau_i(\mathbf{r}, \mathbf{\Omega}, z)$ is the optical distance from the surface point $\mathbf{r}$ to the interior point $\mathbf{r} - z\mathbf{\Omega}$. So the flux at x due to a certain surface flux specified by $(\mathbf{r}, \mathbf{\Omega})$ can be represented by following equation:

$$e^{-\tau_i(\mathbf{r}, \mathbf{\Omega}, l(\mathbf{r}, \mathbf{\Omega}))} \varphi_0^{out}(x - l(\mathbf{r}, \mathbf{\Omega})) f_i(\mathbf{r}, \mathbf{\Omega}) |\mathbf{\Omega} \cdot \hat{n}| d\mathbf{\Omega} dA \ . \tag{114}$$

On the other hand, the neutrons originating from the second source (internal source) travel over the distance z. Thus the neutron at a certain $(\mathbf{r}, \mathbf{\Omega})$ would experience an exponential attenuation determined by the optical distance, $e^{-\tau_i(\mathbf{r}, \mathbf{\Omega}, z)}$. After integrating along the distance z,

the flux at x due to the internal source at $(\mathbf{r}, \boldsymbol{\Omega})$ is obtained as the following:

$$\int_0^{l(\mathbf{r}, \boldsymbol{\Omega})} e^{-\tau_i(\mathbf{r}, \boldsymbol{\Omega}, z)} S_i(\mathbf{r} - z\boldsymbol{\Omega}, \boldsymbol{\Omega}) dz \, f_i(\mathbf{r}, \boldsymbol{\Omega}) |\boldsymbol{\Omega} \cdot \hat{n}| d\boldsymbol{\Omega} dA \tag{115}$$

Finally we can write the outgoing flux at x as following:

$$\varphi_i^{out}(x) = \int_{\Gamma_i^g} \int_{(2\pi)_{out}} \left(e^{-e^{-\tau_i(\mathbf{r}, \boldsymbol{\Omega}, l(\mathbf{r}, \boldsymbol{\Omega}))}} \varphi_0^{out}(x - l(\mathbf{r}, \boldsymbol{\Omega})) + \varphi_i^{out}(\mathbf{r}, \boldsymbol{\Omega}) \right) f_i(\mathbf{r}, \boldsymbol{\Omega}) |\boldsymbol{\Omega} \cdot \hat{n}| d\boldsymbol{\Omega} dA . \tag{116}$$

Here $\varphi_i^{out}(\mathbf{r}, \boldsymbol{\Omega})$ is the exiting flux due to the internal sources along the trajectory $(\mathbf{r}, \boldsymbol{\Omega})$:

$$\varphi_i^{out}(\mathbf{r}, \boldsymbol{\Omega}) = \int_0^{l(\mathbf{r}, \boldsymbol{\Omega})} e^{-\tau_i(\mathbf{r}, \boldsymbol{\Omega}, z)} S_i(\mathbf{r} - z\boldsymbol{\Omega}, \boldsymbol{\Omega}) dz . \tag{117}$$

Note that the source term depends on the local (grain) coordinate, while the average transition flux φ_0^{out} depends on the absolute position on the ray. We now introduce the length chord variable y by simply inserting the identity $\int_0^{L_i} \delta(y - l(\mathbf{r}, \boldsymbol{\Omega})) dy = 1$ inside the $d\boldsymbol{\Omega} dA$ integration in Eq. (116). The $\delta(y)$ is the Kronecker delta function, namely, $\delta(y)$ equal to 1 in $y=0$ and 0 otherwise. So the identity $\int_0^{L_i} \delta(y - l(\mathbf{r}, \boldsymbol{\Omega})) dy = 1$ always holds:

$$
\begin{aligned}
&\varphi_i^{out}(x) \\
&= \int_{\Gamma_i^g} \int_{(2\pi)_{out}} \int_0^{L_i} \delta(y - l(\mathbf{r}, \boldsymbol{\Omega})) dy \Big(e^{-e^{-\tau_i(\mathbf{r}, \boldsymbol{\Omega}, l(\mathbf{r}, \boldsymbol{\Omega}))}} \varphi_0^{out}(x - l(\mathbf{r}, \boldsymbol{\Omega})) \\
&\qquad + \int_0^{l(\mathbf{r}, \boldsymbol{\Omega})} e^{-\tau_i(\mathbf{r}, \boldsymbol{\Omega}, z)} S_i(\mathbf{r} - z\boldsymbol{\Omega}, \boldsymbol{\Omega}) dz \Big) f_i(\mathbf{r}, \boldsymbol{\Omega}) |\boldsymbol{\Omega} \cdot \hat{n}| d\boldsymbol{\Omega} dA \\
&= \int_0^{L_i} \int_{\Gamma_i^g} \int_{(2\pi)_{out}} \Big(\delta(y - l(\mathbf{r}, \boldsymbol{\Omega})) e^{-e^{-\tau_i(\mathbf{r}, \boldsymbol{\Omega}, y)}} \varphi_0^{out}(x - y) \\
&\qquad + H(l(\mathbf{r}, \boldsymbol{\Omega}) - y) e^{-\tau_i(\mathbf{r}, \boldsymbol{\Omega}, y)} S_i(\mathbf{r} - y\boldsymbol{\Omega}, \boldsymbol{\Omega}) \Big) f_i(\mathbf{r}, \boldsymbol{\Omega}) |\boldsymbol{\Omega} \cdot \hat{n}| d\boldsymbol{\Omega} dA dy \\
&= \int_0^{L_i} \Big(\Big\langle \delta(y - l(\mathbf{r}, \boldsymbol{\Omega})) e^{-e^{-\tau_i(\mathbf{r}, \boldsymbol{\Omega}, l(\mathbf{r}, \boldsymbol{\Omega}))}} \Big\rangle_A \varphi_0^{out}(x - y) \\
&\qquad + \Big\langle H(l(\mathbf{r}, \boldsymbol{\Omega}) - y) e^{-\tau_i(\mathbf{r}, \boldsymbol{\Omega}, y)} S_i(\mathbf{r} - y\boldsymbol{\Omega}, \boldsymbol{\Omega}) \Big\rangle_A \Big) dy
\end{aligned}
\tag{118}
$$

where the $H(y)$ is a Heaviside step function, namely, $H(y)$ equal to 1 in $y>0$ and 0 otherwise and $\langle \ \rangle_A$ indicates the integration over the surface Γ_i^g and over $(2\pi)_{out}$ with multiplication by $f_i(\mathbf{r}, \boldsymbol{\Omega}) |\boldsymbol{\Omega} \cdot \hat{n}|$. We are now able to show that our generalization of renewal

processes contains as a limiting case the previous formulation. Indeed, if we assume that the optical thickness and the source in the material depend only on the position along the ray, i.e.

$$\boldsymbol{\tau}_i(\mathbf{r},\boldsymbol{\Omega},y) = \tau_i(x-y,x), \qquad \mathbf{S}_i(\mathbf{r}-y\boldsymbol{\Omega},\boldsymbol{\Omega}) = S_i(x-y), \tag{119}$$

then Eq. (118) reduces to the more familiar form:

$$\varphi_i^{out}(x) = \int_0^{L_i} \left(S_i(x-y)Q_i(y) + \varphi_0^{out}(x-y)f_i(y) \right) e^{-\tau_i(x-y,x)} dy, \tag{120}$$

where

$$f_i(y) = \left\langle \delta\left(y - l(\mathbf{r},\boldsymbol{\Omega})\right) \right\rangle_A, \tag{121}$$

is the probability density for chord of length y. Note that $l(\mathbf{r},\boldsymbol{\Omega})$ is the chord length for the line segment stretching toward $\boldsymbol{\Omega}$ at a surface point $\mathbf{r}$. This analog shows also how to proceed in the more general case when the grains have internal structure. In fact, it suffices to define appropriate averages to reduce Eq. (118) to the familiar form. For instance, we may associate an average optical thickness $\tau_i(y)$ to chords of length y by the expression:

$$f_i(y)e^{-\tau_i(y)} = \left\langle e^{-\boldsymbol{\tau}_i(\mathbf{r},\boldsymbol{\Omega},z)} \delta\left(y - l(\mathbf{r},\boldsymbol{\Omega})\right) \right\rangle_A, \tag{122}$$

and an average source $S_i(y)$ to chords of length greater than y according to:

$$S_i(y)Q_i(y)e^{-\tau_i(y)} = \left\langle e^{-\boldsymbol{\tau}_i(\mathbf{r},\boldsymbol{\Omega},z)} S_i(\mathbf{r}-y\boldsymbol{\Omega},\boldsymbol{\Omega}) H\left(l(\mathbf{r},\boldsymbol{\Omega})-y\right) \right\rangle_A, \tag{123}$$

which effectively allows to rewrite Eq. (118) in the form of Eq. (120). However, in order to deal directly with each different layer in the grain, we choose to write the source contribution in terms of the escape probability. The grain which has internal layers is shown in Figure 9.
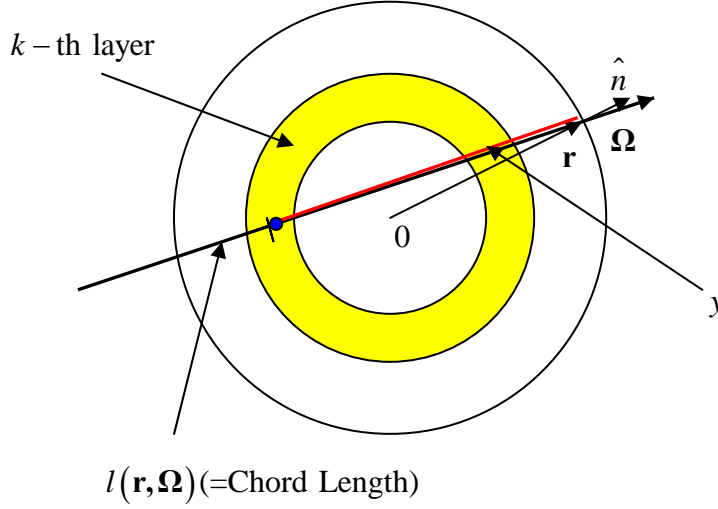
$l(\mathbf{r},\mathbf{\Omega})(=$Chord Length$)$

Figure 9. The heterogeneous grain

Consider a uniform, unity and isotropic neutron distribution within the k-th layer so that the angular source density is 1.0. In order to identify the neutron emitting from layer k within grain type i, introduce a characteristic function $\chi_{ik}(\mathbf{r})$ which is equal to 1 for $\mathbf{r}$ in layer k and 0 otherwise. For a neutron produced at position $\mathbf{r} - y\mathbf{\Omega}$ with direction $\mathbf{\Omega}$, the probability that the neutron will escape from the grain without making a collision is $e^{-\tau_i(\mathbf{r},\mathbf{\Omega},z)}$. For a given surface element dA and a direction $\mathbf{\Omega}$, there can be a pipe line stretched to the interior of the grain along the $-\mathbf{\Omega}$ direction. The cross sectional area of the pipe is $dA' = |\hat{n}\cdot\mathbf{\Omega}|dA$. The volume element at y for dy is thus $dV' = dy|\hat{n}\cdot\mathbf{\Omega}|dA$. Therefore the source given at y for moving toward $d\mathbf{\Omega}$ around $\mathbf{\Omega}$ is $dy|\hat{n}\cdot\mathbf{\Omega}|dAd\mathbf{\Omega}$. For given dA, the integral over the angle should be done only for the outward directions which requires the multiplication of $\pi A_i^g f_i(\mathbf{r},\mathbf{\Omega})$ as discussed below Eq. (113). Noting that there are a total of $4\pi V_{ik}^g$ neutrons emitting from the layer, we can obtain the escape probability:

$$
\begin{aligned}
E_{ik}^g &= \frac{1}{4\pi V_{ik}^g}\int_{\Gamma_i^g}\int_{(2\pi)_{out}}\int_0^{l(\mathbf{r},\mathbf{\Omega})} e^{-\tau_i(\mathbf{r},\mathbf{\Omega},z)}\chi_{ik}(\mathbf{r}-y\mathbf{\Omega})dy|\mathbf{\Omega}\cdot\hat{n}|\pi A_i^g f_i(\mathbf{r},\mathbf{\Omega})dAd\mathbf{\Omega} \\
&= \pi A_i^g\int_{\Gamma_i^g}\int_{(2\pi)_{out}}\varphi_{ik}(\mathbf{r},\mathbf{\Omega})f_i(\mathbf{r},\mathbf{\Omega})|\mathbf{\Omega}\cdot\hat{n}|d\mathbf{\Omega}dA \\
&= \pi A_i^g\left\langle\varphi_{ik}(\mathbf{r},\mathbf{\Omega})\right\rangle_A
\end{aligned}
\tag{124}
$$

where

$$\varphi_{ik}\left(\mathbf{r},\mathbf{\Omega}\right)=\frac{1}{4\pi V_{ik}^g}\int_0^{l(\mathbf{r},\mathbf{\Omega})}e^{-\tau_i(\mathbf{r},\mathbf{\Omega},z)}\chi_{ik}\left(\mathbf{r}-y\mathbf{\Omega}\right)dy\,,\tag{125}$$

is the uncollided flux exiting the grain at $\left(\mathbf{r},\mathbf{\Omega}\right)$ due to a unit isotropic and uniform source in layer k. When the sources within the grain are uniform and isotropic in each layer, then we can use Eqs. (124), (125) and (68) to write the source contribution in Eq. (116) as:

$$
\begin{aligned}
\tilde{\varphi}_i^{out} &= \int_{\Gamma_i^g}\int_{(2\pi)_{out}}\varphi_i^{out}\left(\mathbf{r},\mathbf{\Omega}\right)f_i\left(\mathbf{r},\mathbf{\Omega}\right)\left|\mathbf{\Omega}\cdot\hat{n}\right|d\mathbf{\Omega}dA \\
&= \int_{\Gamma_i^g}\int_{(2\pi)_{out}}\int_0^{l(\mathbf{r},\mathbf{\Omega})}e^{-\tau_i(\mathbf{r},\mathbf{\Omega},z)}S_i\left(\mathbf{r}-z\mathbf{\Omega},\mathbf{\Omega}\right)dzf_i\left(\mathbf{r},\mathbf{\Omega}\right)\left|\mathbf{\Omega}\cdot\hat{n}\right|d\mathbf{\Omega}dA \\
&= \int_{\Gamma_i^g}\int_{(2\pi)_{out}}\int_0^{l(\mathbf{r},\mathbf{\Omega})}e^{-\tau_i(\mathbf{r},\mathbf{\Omega},z)}\sum_k\chi_{ik}\left(\mathbf{r}-z\mathbf{\Omega}\right)S_i\left(\mathbf{r}-z\mathbf{\Omega},\mathbf{\Omega}\right)dzf_i\left(\mathbf{r},\mathbf{\Omega}\right)\left|\mathbf{\Omega}\cdot\hat{n}\right|d\mathbf{\Omega}dA \\
&= \sum_k\int_{\Gamma_i^g}\int_{(2\pi)_{out}}\int_0^{l(\mathbf{r},\mathbf{\Omega})}e^{-\tau_i(\mathbf{r},\mathbf{\Omega},z)}\chi_{ik}\left(\mathbf{r}-z\mathbf{\Omega}\right)S_i\left(\mathbf{r}-z\mathbf{\Omega},\mathbf{\Omega}\right)dzf_i\left(\mathbf{r},\mathbf{\Omega}\right)\left|\mathbf{\Omega}\cdot\hat{n}\right|d\mathbf{\Omega}dA \\
&= \sum_k S_{ik}\int_{\Gamma_i^g}\int_{(2\pi)_{out}}\int_0^{l(\mathbf{r},\mathbf{\Omega})}e^{-\tau_i(\mathbf{r},\mathbf{\Omega},z)}\chi_{ik}\left(\mathbf{r}-z\mathbf{\Omega}\right)dzf_i\left(\mathbf{r},\mathbf{\Omega}\right)\left|\mathbf{\Omega}\cdot\hat{n}\right|d\mathbf{\Omega}dA \\
&= \sum_k S_{ik}\frac{4\pi V_{ik}^g}{\pi A_i^g}E_{ik}^g = \sum_k S_{ik}\frac{4V_i^g}{A_i^g}\frac{V_{ik}^g}{V_i^g} = \overline{l}_i\sum_k p_{ik}^g E_{ik}^g S_{ik}
\end{aligned}
\tag{126}
$$

where we have used the decomposition of unity as $1=\sum_k\chi_{ik}\left(\mathbf{r}\right)$ which is valid in any point within the grain, and where $p_{ik}^g=\dfrac{V_{ik}^g}{V_i^g}$ is the volumetric fraction of layer k in grain i. Note that the above outgoing flux due to the internal source for the heterogeneous case is the generalization of the corresponding one for the homogeneous case given in Eq. (82). Using Eq. (122) to calculate the transition term gives the result:

$$\varphi_i^{out}(x)=\int_0^{L_i}\varphi_0^{out}(x-y)f_i(y)e^{-\tau_i(y)}dy+\tilde{\varphi}_i^{out}\,.\tag{127}$$

This equation is very similar to Eq. (63) and again the solution for the average exiting fluxes is given by Eqs. (80) and (83). The asymptotic flux of Eq. (87) is now modified as the following with the heterogeneous grain source term:

$$\varphi_{as} = \frac{S_0 + \dfrac{1}{\bar{\bar{l}}_0}\sum_i t_i \varphi_i^{out}}{\tilde{\Sigma}_0 - \dfrac{1}{\bar{\bar{l}}_0}\sum_i t_i T_i^g} = \frac{S_0 + \dfrac{1}{\bar{\bar{l}}_0}\sum_i t_i \bar{l}_i \sum_k S_{ik} p_{ik}^g E_{ik}^g}{\Sigma_0 + \dfrac{1}{\bar{\bar{l}}_0} - \dfrac{1}{\bar{\bar{l}}_0}\sum_i t_i T_i^g}$$

$$= \frac{S_0 + \dfrac{1}{p_0}\sum_i p_i \sum_k S_{ik} p_{ik}^g E_{ik}^g}{\Sigma_0 + \dfrac{1}{p_0}\sum_i \dfrac{p_i}{\bar{l}_i}(1-T_i^g)} = \frac{1}{\tilde{\Sigma}}\left(S_0 + \frac{1}{p_0}\sum_i p_i \sum_k S_{ik} p_{ik}^g E_{ik}^g \right)$$

(128)

Also, all the coefficients depending on the XS of the grain must be modified to account for the internal structure. In particular, Eq. (82) are replaced by:

$$T_i^g = \int_0^{L_i} e^{-\tau_i(y)} f_i(y)dy = \left\langle e^{-\tau_i(\mathbf{r},\mathbf{\Omega})} \right\rangle_A ,$$
$$\hat{T}_i^g = \int_0^{L_i} e^{-\tau_i(y)+\Sigma y} f_i(y)dy = \left\langle e^{-\tau_i(\mathbf{r},\mathbf{\Omega})+\Sigma l(\mathbf{r},\mathbf{\Omega})} \right\rangle_A$$

(129)

while Eqs. (102) and (103) are modified using Eq. (30) to:

$$\tilde{\Sigma} = \Sigma_0 + \frac{1}{\bar{\bar{l}}_0}\sum_{i=1}^N t_i\left(1-T_i^g\right) = \Sigma_0 + \frac{1}{p_0}\sum_{i=1}^N \frac{p_i}{\bar{l}_i}\left(1-T_i^g\right)$$

$$= \Sigma_0 + \frac{1}{p_0}\sum_{i=1}^N p_i \sum_{k=1}^K p_{ik}^g \Sigma_{ik} E_{ik}^g = \Sigma_0 + \frac{1}{p_0}\sum_{i=1}^N \sum_{k=1}^K p_{ik}\Sigma_{ik} E_{ik}^g$$

(130)

$$\Sigma = \Sigma_0 + \frac{1}{p_0}\sum_{i=1}^N \sum_{k=1}^K p_{ik}(\Sigma_{ik}-\Sigma)\hat{E}_{ik}^g(\Sigma) .$$

(131)

Note again that Eq. (131) implicitly defines the effective cross section for the mixture. It should be solved iteratively.

6.3 Interior Flux

The equation for the interior flux $\varphi_i(x)$ is also obtained in a similar manner. By using the density of probability, $g_i(\mathbf{r},\mathbf{\Omega})$, we can write an equation for the average flux at x when this point is in layer k of a grain of type i. There are also two contributions in this case if $\varphi_i(x)$ is for the average angular flux in grain i at x. The first one is due to the surface source and the

other one is due to the interior source. Let's denote the position of the first source by $x - l(\mathbf{r}, \mathbf{\Omega})$ in the absolute coordinate and the second source by $\mathbf{r} - z\mathbf{\Omega}$ in the relative coordinate as shown below.
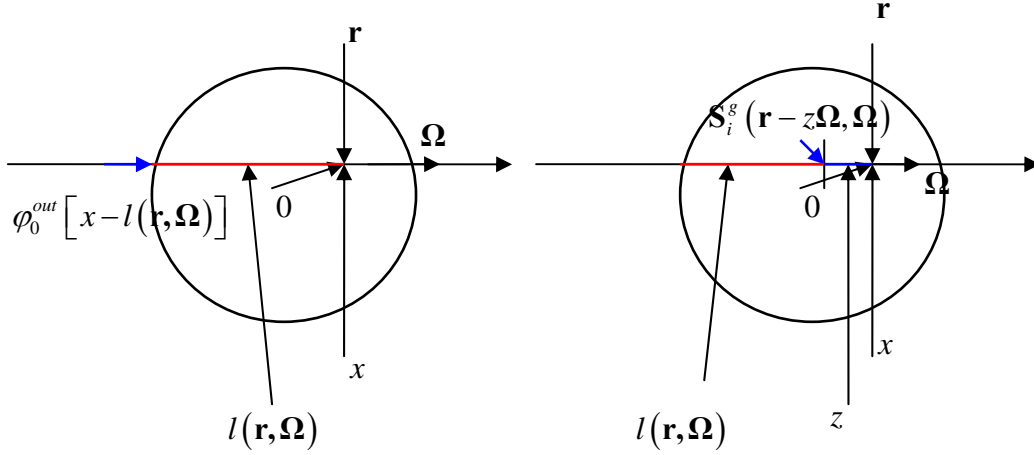

Figure 10. Two sources contributing to $\varphi_i(x)$

After traveling the distance $l(\mathbf{r}, \mathbf{\Omega})$ from the first source (incoming source), the neutrons at a certain $(\mathbf{r}, \mathbf{\Omega})$ would experience an exponential attenuation determined by the optical distance, $e^{-\tau_i(\mathbf{r}, \mathbf{\Omega}, l(\mathbf{r}, \mathbf{\Omega}))}$. So the flux at x in a certain $(\mathbf{r}, \mathbf{\Omega})$ would be:

$$e^{-\tau_i(\mathbf{r}, \mathbf{\Omega}, l(\mathbf{r}, \mathbf{\Omega}))} \varphi_0^{out}\left(x - l(\mathbf{r}, \mathbf{\Omega})\right) g_i(\mathbf{r}, \mathbf{\Omega}) dV d\mathbf{\Omega} \tag{132}$$

On the other hand, the second source (internal source) travels over the distance z and the neutrons at a certain $(\mathbf{r}, \mathbf{\Omega})$ would experience an exponential attenuation determined by the optical distance, $e^{-\tau_i(\mathbf{r}, \mathbf{\Omega}, z)}$. After integrating along the distance z, the flux would be:

$$\int_0^{l(\mathbf{r}, \mathbf{\Omega})} e^{-\tau_i(\mathbf{r}, \mathbf{\Omega}, z)} S_i(\mathbf{r} - z\mathbf{\Omega}, \mathbf{\Omega}) dz \, g_i(\mathbf{r}, \mathbf{\Omega}) d\mathbf{\Omega} dV \tag{133}$$

Finally we can write the flux at x as the following:

$$\varphi_{ik}(x)$$
$$= \int_{V_i^g} \int_{4\pi} \chi_{ik}(\mathbf{r}) \left(e^{-\tau_i(\mathbf{r},\Omega,l(\mathbf{r},\Omega))} \varphi_0^{out}(x - l(\mathbf{r},\Omega)) + \varphi_i(\mathbf{r},\Omega) \right) \frac{g_i(\mathbf{r},\Omega)}{p_{ik}^g} d\Omega d\mathbf{r} \tag{134}$$

where $l(\mathbf{r},\Omega)$ is the distance in direction $-\Omega$ from the point $\mathbf{r}$ to the surface of the grain (distance to the point at which the trajectory enters the surface of the grain), $\varphi_i(\mathbf{r},\Omega)$ is the contribution of the internal sources to the flux at $(\mathbf{r},\Omega)$, namely:

$$\varphi_i(\mathbf{r},\Omega) = \int_0^{l(\mathbf{r},\Omega)} e^{-\tau_i(\mathbf{r},\Omega,z)} S_i(\mathbf{r} - z\Omega,\Omega) dz, \tag{135}$$

and $\tau_i(\mathbf{r},\Omega,z)$ is the optical thickness from point $\mathbf{r}$ to point $\mathbf{r} - z\Omega$. The characteristic function χ_{ik} in Eq. (134) is introduced to perform the integral only at the k-th layer and the PDF is divided by the layer volume fraction defined by:

$$p_{ik}^g = \int_{V_i^g} \int_{4\pi} \chi_{ik}(\mathbf{r}) g_i(\mathbf{r},\Omega) d\Omega d\mathbf{r} \tag{136}$$

in order to reflect that the original PDF is defined for the whole grain, not just for the layer. Renormalization is thus necessary to make the new PDF sums up to 1.0.

As before we introduce the length along the trajectory y by inserting $\int_0^{L_i} \delta(y - l(\mathbf{r},\Omega)) dy$ inside the $d\Omega d\mathbf{r}$ in Eq. (134). After bringing the integration over dy out to the outside, we obtain an expression very similar to Eq. (118), namely:

$$p_{ik}^g \varphi_{ik}(x)$$
$$= \int_{V_i^g} \chi_{ik}(\mathbf{r}) \int_{4\pi} \int_0^{L_i} \delta(y - l(\mathbf{r},\Omega)) dy \left(e^{-e^{-\tau_i(\mathbf{r},\Omega,l(\mathbf{r},\Omega))}} \varphi_0^{out}(x - l(\mathbf{r},\Omega)) \right.$$
$$\left. + \int_0^{l(\mathbf{r},\Omega)} e^{-\tau_i(\mathbf{r},\Omega,z)} S_i(\mathbf{r} - z\Omega,\Omega) dz \right) g_i(\mathbf{r},\Omega) d\Omega dV$$
$$= \int_0^{L_i} \int_{V_i^g} \int_{4\pi} \left(\chi_{ik}(\mathbf{r}) \delta(y - l(\mathbf{r},\Omega)) e^{-e^{-\tau_i(\mathbf{r},\Omega,y)}} \varphi_0^{out}(x - y) \right.$$
$$\left. + \chi_{ik}(\mathbf{r}) H(l(\mathbf{r},\Omega) - y) e^{-\tau_i(\mathbf{r},\Omega,y)} S_i(\mathbf{r} - y\Omega,\Omega) \right) g_i(\mathbf{r},\Omega) d\Omega dV dy \tag{137}$$

$$
= \int_0^{L_i} \left(\left\langle \chi_{ik}(\mathbf{r}) \delta(y - l(\mathbf{r},\mathbf{\Omega})) e^{-e^{-\tau_i(\mathbf{r},\mathbf{\Omega},l(\mathbf{r},\mathbf{\Omega}))}} \right\rangle_V \varphi_0^{out}(x-y) \right.
$$
$$
\left. + \left\langle \chi_{ik}(\mathbf{r}) H(l(\mathbf{r},\mathbf{\Omega}) - y) e^{-\tau_i(\mathbf{r},\mathbf{\Omega},y)} S_i(\mathbf{r} - y\mathbf{\Omega},\mathbf{\Omega}) \right\rangle_V \right) dy
$$

Now $\langle \ \rangle_V$ indicates the integration over the grain volume V_i^g and solid angle (4π) after multiplication by $g_i(\mathbf{r},\mathbf{\Omega})$. Noting that $4\pi V_i^g$ should be multiplied to $g_i(\mathbf{r},\mathbf{\Omega})$ to merely select the phase point where $g_i(\mathbf{r},\mathbf{\Omega}) \neq 0$. We define the collision probability as the following in order to account for the contribution from the sources of each layer:

$$
P_{ik,il}^g = \Sigma_{ik} \int_{V_i^g} \int_{4\pi} \chi_{ik}(\mathbf{r}) \frac{1}{4\pi V_{il}^g} \int_0^{l(\mathbf{r},\mathbf{\Omega})} e^{-\tau_i(\mathbf{r},\mathbf{\Omega},y)} \chi_{il}(\mathbf{r} - y\mathbf{\Omega}) dy 4\pi V_i^g g_i(\mathbf{r},\mathbf{\Omega}) d\mathbf{\Omega} d\mathbf{r} \quad (138)
$$
$$
= 4\pi V_i^g \Sigma_{ik} \int_{V_i^g} \int_{4\pi} \chi_{ik}(\mathbf{r}) \frac{1}{4\pi V_{il}^g} \int_0^{l(\mathbf{r},\mathbf{\Omega})} e^{-\tau_i(\mathbf{r},\mathbf{\Omega},y)} \chi_{il}(\mathbf{r} - y\mathbf{\Omega}) dy g_i(\mathbf{r},\mathbf{\Omega}) d\mathbf{\Omega} d\mathbf{r}
$$
$$
= 4\pi V_i^g \Sigma_{ik} \int_{V_i^g} \int_{4\pi} \chi_{ik}(\mathbf{r}) \varphi_{il}(\mathbf{r},\mathbf{\Omega}) g_i(\mathbf{r},\mathbf{\Omega}) d\mathbf{\Omega} d\mathbf{r}
$$
$$
= 4\pi V_i^g \Sigma_{ik} \left\langle \chi_{ik}(\mathbf{r}) \varphi_{il}(\mathbf{r},\mathbf{\Omega}) \right\rangle_V
$$

where $\varphi_{il}(\mathbf{r},\mathbf{\Omega})$ is the uncollided flux at $(\mathbf{r},\mathbf{\Omega})$ due to a unit isotropic and uniform source in layer l. This flux is obtained from Eq. (125) by merely replacing ik with il. The difference now is that $(\mathbf{r},\mathbf{\Omega})$ is an interior point in the grain and that $l(\mathbf{r},\mathbf{\Omega})$ is the length of the trajectory from the entering point on surface Γ_i^g to point $\mathbf{r}$. With these definitions, we can write the volumetric source contribution to $\varphi_{ik}(x)$ in Eq. (137) as the following:

$$
\varphi_{ik} = \frac{1}{p_{ik}^g} \int_{V_i^g} \chi_{ik}(\mathbf{r}) \int_{4\pi} \int_0^{l(\mathbf{r},\mathbf{\Omega})} e^{-\tau_i(\mathbf{r},\mathbf{\Omega},z)} S_i(\mathbf{r} - z\mathbf{\Omega},\mathbf{\Omega}) dz g_i(\mathbf{r},\mathbf{\Omega}) d\mathbf{\Omega} dV \quad (139)
$$
$$
= \frac{1}{p_{ik}^g} \int_{V_i^g} \chi_{ik}(\mathbf{r}) \int_{4\pi} \int_0^{l(\mathbf{r},\mathbf{\Omega})} e^{-\tau_i(\mathbf{r},\mathbf{\Omega},z)} \sum_l \chi_{il}(\mathbf{r} - z\mathbf{\Omega}) S_i(\mathbf{r} - z\mathbf{\Omega},\mathbf{\Omega}) dz g_i(\mathbf{r},\mathbf{\Omega}) d\mathbf{\Omega} dV
$$
$$
= \frac{1}{p_{ik}^g} \sum_l S_{il} \int_{V_i^g} \chi_{ik}(\mathbf{r}) \int_{4\pi} \int_0^{l(\mathbf{r},\mathbf{\Omega})} e^{-\tau_i(\mathbf{r},\mathbf{\Omega},z)} \chi_{il}(\mathbf{r} - z\mathbf{\Omega}) dz g_i(\mathbf{r},\mathbf{\Omega}) d\mathbf{\Omega} dV
$$
$$
= \frac{1}{p_{ik}^g} \frac{1}{V_i^g \Sigma_{ik}} \sum_l V_{il}^g S_{il} P_{ik,il}^g
$$
$$
= \frac{1}{V_{ik}^g \Sigma_{ik}} \sum_l V_{il}^g S_{il} P_{ik,il}^g
$$

To account for the contribution from the interface flux $\varphi_0^{out}(x-y)$ we introduce an average

optical path for each layer as:

$$g_i(y)e^{-\tau_{ik}(y)} = \left\langle \chi_{ik}(\mathbf{r})e^{-\tau_i(\mathbf{r},\mathbf{\Omega},y)}\delta(y - l(\mathbf{r},\mathbf{\Omega})) \right\rangle_V \tag{140}$$

where $g_i(y)$ is the density of probability that, given that the point x is inside grain i, the distance of the trajectory from the entering point to x is y, i.e.

$$g_i(y) = \left\langle \delta(y - l(\mathbf{r},\mathbf{\Omega})) \right\rangle_V . \tag{141}$$

Putting the two contributions (volumetric and surface) together we have:

$$\varphi_{ik}(x) = \frac{1}{p_{ik}^g}\int_0^{L_i} e^{-\tau_{ik}(y)} g_i(y)\varphi_0^{out}(x - y)dy + \varphi_{ik} \tag{142}$$

Therefore, use of solution (91) yields the result:

$$\varphi_{ik}(x) = \varphi_0(0)\hat{E}_{ik}^g e^{-\Sigma x} + \varphi_{as}(E_{ik}^g - \hat{E}_{ik}^g e^{-\Sigma x}) + \varphi_{ik} . \tag{143}$$

The escape probabilities in this formula are given in terms of the density $g_i(y)$ as:

$$E_{ik}^g = \frac{1}{p_{ik}^g}\int_0^{L_i} e^{-\tau_{ik}(y)} g_i(y)dy = \left\langle \chi_{ik}(\mathbf{r})e^{-\tau_i(\mathbf{r},\mathbf{\Omega})} \right\rangle_V \tag{144}$$
$$\hat{E}_{ik}^g = \frac{1}{p_{ik}^g}\int_0^{L_i} e^{-\tau_{ik}(y)+\Sigma y} g_i(y)dy = \left\langle \chi_{ik}(\mathbf{r})e^{-\tau_i(\mathbf{r},\mathbf{\Omega})+\Sigma l(\mathbf{r},\mathbf{\Omega})} \right\rangle_V$$

where $\tau_i(\mathbf{r},\mathbf{\Omega}) = \tau_i(\mathbf{r},\mathbf{\Omega},l(\mathbf{r},\mathbf{\Omega}))$ is the optical distance in direction $-\mathbf{\Omega}$ from point $\mathbf{r}$ to the surface Γ_i^g.

With the definitions of the layer escape probabilities, the layer average angular flux corresponding to the homogeneous case, Eq. (105) becomes now

$$\overline{\varphi}_{ik} = \overline{\varphi}_0\hat{E}_{ik}^g + \varphi_{as}(E_{ik}^g - \hat{E}_{ik}^g) + \frac{1}{V_{ik}^g\Sigma_{ik}}\sum_l V_{il}^g S_{il} P_{ik,il}^g . \tag{145}$$

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and the peudo cross section needed for the renormaliztion, Eq. (107), is now

$$\hat{\Sigma} = p_0 \Sigma_0 + \sum_{i=1}^{N} \sum_{k=1}^{K} p_{ik} \Sigma_{ik} \hat{E}_{ik}^g \; . \tag{146}$$

Noting that Eq. (131) can be rewritten as:

$$\Sigma \left(p_0 + \sum_{i=1}^{N} \sum_{k=1}^{K} p_{ik} \hat{E}_{ik}^g (\Sigma) \right) = p_0 \Sigma_0 + \sum_{i=1}^{N} \sum_{k=1}^{K} p_{ik} \Sigma_{ik} \hat{E}_{ik}^g = \hat{\Sigma} \tag{147}$$

we can represent the peusdo cross section in a simpler way as:

$$\hat{\Sigma} = r \Sigma \tag{148}$$

where the renormalization factor is defined as:

$$r = p_0 + \sum_{i=1}^{N} \sum_{k=1}^{K} p_{ik} \hat{E}_{ik}^g (\Sigma) \; . \tag{149}$$

7. Calculation Sequence for MOC with Double Heterogeneity

By integrating the MOC solution and the analytic solution for the heterogeneous grain, we can now set the calculation sequence for the stochastic medium as the following:

1) calculate the collision probabilities and escape probabilities corresponding to Eqs. (138) and (144) for the grains given the cross sections and geometry

2) determine $\hat{E}_{ik}^{g}$ and Σ iteratively, by Eq. (131) and Eq. (144)

3) calculate β by Eq. (98) and r by Eq.(149), and $\hat{\beta} = r\beta$

4) set the source in the matrix and each grain layer and obtain the asymptotic flux φ_{as} by Eq. (128) and then the effective source for MOC by multiplying φ_{as} by Σ

5) update the matrix and grain layer average angular flux by Eqs. (104) and (105), and accumulate each scalar flux

6) determine FSR-outgoing current by Eq. (109)

7) move to the next FSR by using the outgoing current of the previous region

8) update matrix and grain sources using the scalar flux after the ray sweep is done for all angles

9) repeat the MOC-DH iterations (Steps 4-9) until the flux converges

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