Design for the MC simulation

The block diagram of the both spectral and diffuse reflections is given on the next page. This system considers the parameters of emissivity (solid absorptivity), refractive index, spectral or diffuse reflection of the particles. The parameters of bed length or dimensions, diameter, porosity will be accounted in the model of the porous bed. These algorithms will be run for different values of dimensions, diameter, different size spheres and porosity to get data on all these parameters for training the NN model.

Different equations that will be used in this model include:

Snell's Law

$$\theta_t = \sin^{-1}\left[\frac{n_1 \sin\theta_i}{n_2}\right]$$

Fresnel's Law

$$\rho_{\parallel} = \frac{\tan(\theta_i - \theta_t)}{\tan(\theta_i + \theta_t)}, \quad \rho_{\perp} = \frac{\sin(\theta_i - \theta_t)}{\sin(\theta_i + \theta_t)}$$

$$t_{\parallel} = \frac{2\sin\theta_t\cos\theta_i}{\sin(\theta_i + \theta_t)\cos(\theta_i - \theta_t)}, \quad t_{\perp} = \frac{2\sin\theta_t\cos\theta_i}{\sin(\theta_i + \theta_t)}$$

Now average of parallel and perpendicular components is calculated by adding square of these values and dividing by 2.

$$\rho_{avg} = \left(\rho_{\parallel}^2 + \rho_{\perp}^2\right)/2$$

$$t_{avg} = \left(t_{\parallel}^2 + t_{\perp}^2\right)/2$$

As mentioned in the block diagram, Now this average is compared with the random generated number which decides whether the ray will be refracted or reflected.

$$R_s < \rho_{avg}$$

Spectral Reflection

Direction cosines of the reflected ray are given by laws of reflection. The equation for the direction cosines is:

$$u'_j = u_j - 2n_j \sum_{k=1}^{3} n_k u_k, \quad j = 1, 2, 3$$

Diffuse Reflection

First, we set a local reference frame (x',y',z') with origin at the center od the sphere and z' aligned along the line joining the center and the point of interaction. Now let I', j', k' be the unit vectors along x',y',z' and so these are given by:

$$\mathbf{k}' = \frac{(x_i - x_c)\mathbf{i} + (y_i - y_c)\mathbf{j} + (z_i - z_c)\mathbf{k}}{\sqrt{(x_i - x_c)^2 + (y_i - y_c)^2 + (z_i - z_c)^2}}; \quad \mathbf{i}' = \mathbf{k}' \times \mathbf{k};$$

$$\mathbf{j}' = \mathbf{k}' \times \mathbf{i}'$$

Now for diffuse reflection the reflected ray goes in a random direction and so the direction cosines of the reflected ray are calculated from random variables given as:

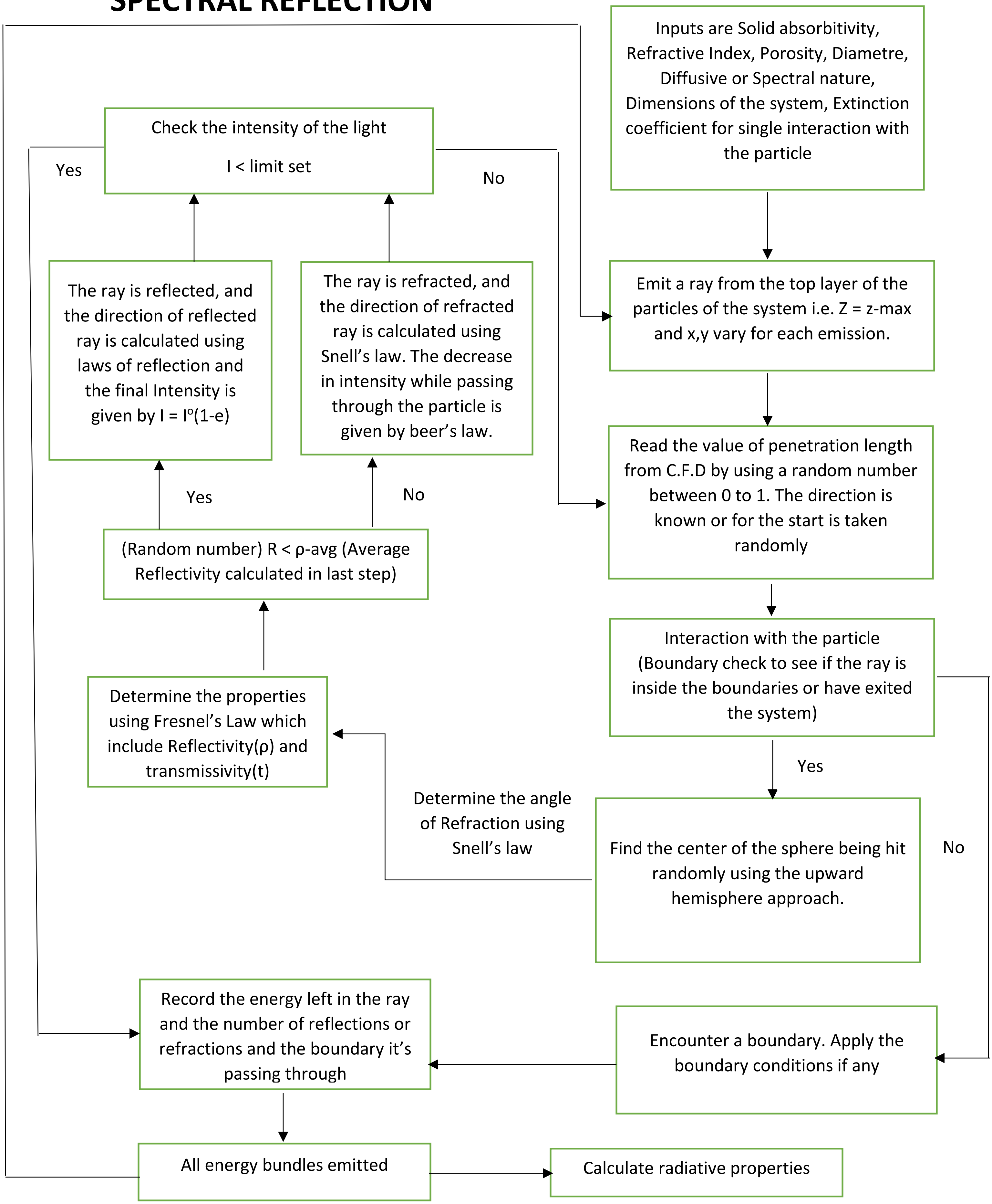
$$\phi' = \sin^{-1}(\sqrt{\xi_3}); \quad \theta' = 2\pi\xi_4$$

$$\mu'_x = \sin\phi' \cos\theta'; \quad \mu'_y = \sin\phi' \sin\theta'; \quad \mu'_z = \cos\phi'$$

Finally, these direction cosines are marked back to the original coordinate system using the rotation matrix given as:

$$\begin{Bmatrix} \mu_x \\ \mu_y \\ \mu_z \end{Bmatrix} = \begin{bmatrix} i'_x & j'_x & k'_x \\ i'_y & j'_y & k'_y \\ i'_z & j'_z & k'_z \end{bmatrix} \begin{Bmatrix} \mu'_x \\ \mu'_y \\ \mu'_z \end{Bmatrix}$$

SPECTRAL REFLECTION



DIFFUSE REFLECTION