CHAPTER II
THEORY OF EXTINCTION AND SCATTERING

2.0. General introduction.

The required theory for processing the data of the air quality monitoring system is developed in this chapter. Section 2.1 begins with the Maxwell equations in order to present the Poynting vector in a form required for developing the Stoke's parameters. Next the relation between incident and scattered fields and the Stoke's parameters are developed. Finally this relation and the Stoke's parameters lead to the formation of the Mueller matrix for scattering, an element of which is monitored by the air quality monitoring system. In Section 2.2 the cross-sections of extinction, absorption and scattering are derived and are then used in forming the theory for extinction co-efficient which is a parameter that is measured by the air quality monitoring system. Since in the experiments with the air quality monitoring system water droplets, which are considered as spherical particles, are investigated, Mie theory is taken up in Section 2.3 to explain the angular variations of the scattered light, as the theory has successfully explained a host of scattering observations done with spherical particles. Finally Section 2.4 gives a method in the form of a computer program to calculate theoretical values of scattering coefficients over size distributions which may be co-related with experimental results. Thus the chapter incorporates the original efforts in the thesis at computerization of the scattering matrix in a format compatible with the design of the air quality monitoring system together with the casting of the standard theory of scattering coefficients in a form that is convenient for computerization.
2.1 Scattering matrix and scattering coefficients

The Maxwell equations [44,31,10] for the electromagnetic field in a region where free charge density \( \rho_f = 0 \) and current density \( J_f = 0 \) are given as

\[
\begin{align*}
\nabla \cdot E &= 0 \quad 2.1.1 \\
\nabla \times E &= -\mu \left( \frac{\partial H}{\partial t} \right) \quad 2.1.2 \\
\nabla \cdot H &= 0 \quad 2.1.3 \\
\nabla \times H &= \varepsilon \left( \frac{\partial E}{\partial t} \right) \quad 2.1.4
\end{align*}
\]

where \( \mu \) and \( \varepsilon \) are the permeability and permittivity respectively of the medium. Hence it follows that if the refractive index of the medium is given as \( n = n' + in'' \), then

\[
E = E_0 e^{-i k' x} e^{i \omega t} \quad 2.1.5
\]

\[
H = H_0 e^{-i k'' x} e^{i \omega t} \quad 2.1.6
\]

where \( k = k' + ik'' \) and \( \omega \) are the wave vector and angular frequency respectively and the Poynting vector \( S \) is given as

\[
S = (1/2) \text{Re} \left\{ (\varepsilon/\mu)^{1/2} (E^* E) \right\} \hat{\varepsilon} \quad 2.1.7
\]

where \( E^* \) is the complex conjugate of \( E \) and \( \hat{\varepsilon} \) is the direction of propagation. Assuming the wave with wavelength \( \lambda \) to be moving in the \( z \) direction, the above equation becomes

\[
S = (k/2\omega \mu) |E_0|^2 e^{-4\pi n' z/\lambda} \hat{\varepsilon} \quad 2.1.8
\]

This gives the modulus of \( S \) as

\[
|S| = (k/2\omega \mu) \quad 2.1.9
\]
where $I$ is the irradiance with dimension of energy per unit area and time. As the wave traverses the medium, the irradiance may be given from 2.1.8 and 2.1.9 as,

$$I = I_0 e^{-\alpha' z} \quad 2.1.10$$

where

$$\alpha' = 4\pi n''/\lambda \quad 2.1.11$$

is the absorption co-efficient and

$$I_o = (k/2\omega\mu)|E_o|^2 \quad 2.1.12$$

is the irradiance at $z = 0$. Also if there is no absorption in the medium then $n'' = 0$ and 2.1.9 becomes

$$|S| = (k/2\omega\mu)I_o \quad 2.1.13$$

The equations 2.1.12 and 2.1.13 are now in a form that can be used for development of the Stokes parameters which in turn is to be used in developing the Mueller matrix for scattering.
Since the relation between the incident and scattered fields is also required in the development of the Mueller matrix for scattering it is derived by taking the case of scattering by a single particle as shown in figure 2.1. The direction of propagation of the incident light is taken as the \( z \)-axis. Any point in the particle is chosen as the origin of a rectangular Cartesian co-ordinate system \((x,y,z)\), where \( x \) and \( y \) axes are orthogonal to the \( z \)-axis and to each other but are otherwise arbitrary. The orthogonal basis vectors \( \hat{e}_x, \hat{e}_y, \hat{e}_z \) are in the directions of the positive \( x, y \) and \( z \) axes. The direction of scattering may also be given in terms of \( \hat{e}_r, \hat{e}_\theta \) and \( \hat{e}_\phi \) which are the orthonormal basis vectors associated with the spherical polar co-ordinate system \((r, \theta, \phi)\). Here \( \theta \) is the scattering angle and \( \hat{e}_r \) and \( \hat{e}_z \) define the scattering plane. The scattering plane is uniquely determined by the azimuthal angle \( \phi \) except when \( \hat{e}_r \) is parallel to the \( z \)-axis. In these two instances, that is \( \hat{e}_r = \pm \hat{e}_z \), any plane containing the \( z \)-axis is a suitable scattering plane. The incident field \( E_i \) which lies in the \( x-y \) plane may now be resolved into components parallel \( E_{i||} \) and perpendicular \( E_{i\perp} \) to the scattering plane leading to the relation

\[
E_i = (E_{i||}\hat{e}_{||} + E_{i\perp}\hat{e}_{\perp}) e^{i(kz-\omega t)} = E_{i||}\hat{e}_{||} + E_{i\perp}\hat{e}_{\perp} \tag{2.1.14}
\]

also,

\[
\hat{e}_{\perp} = \sin\phi \hat{e}_x - \cos\phi \hat{e}_y \tag{2.1.15}
\]

\[
\hat{e}_{||} = \cos\phi \hat{e}_x + \sin\phi \hat{e}_y \tag{2.1.16}
\]

\[
\hat{e}_{||} \times \hat{e}_{||} = \hat{e}_z \tag{2.1.17}
\]

\[
\hat{e}_{\perp} = -\hat{e}_\phi \tag{2.1.18}
\]

\[
\hat{e}_{||} = \sin\theta \hat{e}_r + \cos\theta \hat{e}_\theta \tag{2.1.19}
\]

The \( x \) and \( y \) components of \( E_i \) may be denoted by \( E_{ix} \) and \( E_{iy} \). Thus we get

The x and y components of $E_i$ may be denoted by $E_{ix}$ and $E_{iy}$. Thus we get
In the far field region ($kr >> 1$) the scattered field $E_s$ is approximately transverse ($\hat{e}_r, E_s = 0$) and has the asymptotic form [31]

$$E_s \sim (e^{ikr} - ikr)A$$ \hspace{1cm} 2.1.22

where $\hat{e}_r A = 0$ and $A$ is the $\phi$ and $\theta$ dependent vectorial scattering amplitude. Again $E_s$ in the far field region can be written as

$$E_s = E_{||s} \hat{e}_{||s} + E_{\perp s} \hat{e}_{\perp s}$$ \hspace{1cm} 2.1.23

also,

$$\hat{e}_{||s} = \hat{e}_\theta$$ \hspace{1cm} 2.1.24

$$\hat{e}_{\perp s} = -\hat{e}_\phi$$ \hspace{1cm} 2.1.25

$$\hat{e}_{\perp s} \times \hat{e}_{||s} = \hat{e}_r$$ \hspace{1cm} 2.1.26

where the basis vectors $\hat{e}_{||s}$ and $\hat{e}_{\perp s}$ are parallel and perpendicular to the scattering plane respectively. Thus considering the equations 2.1.14 to 2.1.26 the required relation between incident and scattered fields in matrix form may be given as

$$\begin{pmatrix} E_{||s} \\ E_{\perp s} \end{pmatrix} = \frac{e^{ik(r-z)}}{-ikr} \begin{pmatrix} S_2 & S_3 \\ S_4 & S_1 \end{pmatrix} \begin{pmatrix} E_{||s} \\ E_{\perp s} \end{pmatrix}$$ \hspace{1cm} 2.1.27

where the matrix elements $S_j (j=1,2,3,4)$ depends on $\theta$ and $\phi$ and the matrix is the amplitude scattering matrix.

In order to derive the Stoke's parameters a series of hypothetical experiments which can be performed with an arbitrary monochromatic beam, a detector, and
various polarizers, as shown in figure 2.2, in a non-absorbing medium, are considered. The detector responds to irradiance independently of the polarization state, and the polarizers are assumed to be ideal. The electric field \( \mathbf{E} \) is referred to orthogonal axes \( \hat{e}_\parallel \) and \( \hat{e}_\perp \), which is called horizontal and vertical respectively, and \( \mathbf{E}_o \) is given as

\[
\mathbf{E}_o = \mathbf{E}_\parallel \hat{e}_\parallel + \mathbf{E}_\perp \hat{e}_\perp
\]  \hspace{1cm} 2.1.28

Case 1: With no polarizers. If there is no polarizer in the beam the irradiance \( I \) recorded by the detector is given by

\[
I = I_\parallel + I_\perp
\]  \hspace{1cm} 2.1.29

or using 2.1.12 and 2.1.13 by,

\[
I = (k/2\omega \mu_0)(E_\parallel |E_\parallel|^* + E_\perp |E_\perp|^*)
\]  \hspace{1cm} 2.1.30

Case 2: With horizontal and vertical Polarizers. Let \( P \), in figure 2.2, be a horizontal polarizer, the amplitude of the transmitted wave is \( \mathbf{E}_\parallel \) and the irradiance \( I_\parallel \) recorded by the detector is \( (k/2\omega \mu_0)(E_\parallel |E_\parallel|^* \mathbf{E}_\perp |E_\perp|^*) \). Next let \( P \) be a vertical polarizer; the amplitude of the transmitted wave is \( \mathbf{E}_\perp \) and the irradiance \( I_\perp \) recorded by the detector is \( \mathbf{E}_\perp |E_\perp|^* \). The difference between these two measured irradiances is

\[
I_\parallel - I_\perp = (k/2\omega \mu_0)(E_\parallel |E_\parallel|^* - \mathbf{E}_\perp |E_\perp|^*)
\]  \hspace{1cm} 2.1.31
Case 3: $+45^\circ$ and $-45^\circ$ polarizers.

Figure 2.3

An orthonormal set of basis vectors $\mathbf{e}_+$ and $\mathbf{e}_-$, which are obtained by rotating $\mathbf{e}_\parallel$ by $+45^\circ$ and $-45^\circ$, as shown in figure 2.3 may be introduced. Then since,

$$E_+ = (1/2)^{1/2}(E_\parallel + E_\perp) \quad 2.1.32$$

$$E_- = (1/2)^{1/2}(E_\parallel - E_\perp) \quad 2.1.33$$

Therefore electric field $E_0$ may be written as

$$E_0 = E_+\mathbf{e}_+ + E_-\mathbf{e}_- \quad 2.1.34$$

where,

$$E_+ = (1/2)^{1/2}(E_\parallel + E_\perp) \quad 2.1.35$$

$$E_- = (1/2)^{1/2}(E_\parallel - E_\perp) \quad 2.1.36$$

Now if $P$ in figure 2.2 is a $+45^\circ$ polarizer then the amplitude of the transmitted wave is

$$(\kappa/2\omega\mu_0)(E_\parallel E_\parallel^* + E_\parallel E_\perp^* + E_\perp E_\parallel^* + E_\perp E_\perp^*)/2 \quad 2.1.37$$

Again if $P$ is a $-45^\circ$ polarizer then the irradiance of the transmitted wave is

$$I = (\kappa/2\omega\mu_0)(E_\parallel E_\parallel^* - E_\parallel E_\perp^* - E_\perp E_\parallel^* + E_\perp E_\perp^*)/2 \quad 2.1.38$$

The difference between these two irradiances is
Case 4: With circular polarizers. Another set of basis vectors \( \hat{e}_R \) and \( \hat{e}_L \) are defined as

\[
\hat{e}_R = \left( \frac{1}{2} \right)^{1/2} (\hat{e}_\parallel + i\hat{e}_\perp) \tag{2.1.40}
\]

\[
\hat{e}_L = \left( \frac{1}{2} \right)^{1/2} (\hat{e}_\parallel - i\hat{e}_\perp) \tag{2.1.41}
\]

These basis vectors represent right-circularly and left-circularly polarized waves and are orthonormal in the sense that \( \hat{e}_R \cdot \hat{e}_R^* = 1, \hat{e}_L \cdot \hat{e}_L^* = 1, \hat{e}_R \cdot \hat{e}_L^* = 0 \) and \( \hat{e}_L \cdot \hat{e}_R^* = 0 \).

Hence, the incident field may be written as

\[
E_0 = E_R \hat{e}_R + E_L \hat{e}_L \tag{2.1.42}
\]

where,

\[
E_R = \left( \frac{1}{2} \right)^{1/2} (E_\parallel - iE_\perp) \tag{2.1.43}
\]

\[
E_L = \left( \frac{1}{2} \right)^{1/2} (E_\parallel + iE_\perp) \tag{2.1.44}
\]

Now if \( P \) is a right-handed polarizer, then the transmitted irradiance \( I_R \) is

\[
I_R = \frac{k/2 \omega \mu_d}{(k/2 \omega \mu_d)^2} \left( E_\parallel^* \hat{e}_R + E_\perp^* \hat{e}_L \right) / 2 \tag{2.1.45}
\]

Again if \( P \) is a left-handed polarizer, then the transmitted irradiance \( I_L \) is

\[
I_L = \frac{k/2 \omega \mu_d}{(k/2 \omega \mu_d)^2} \left( E_\parallel^* \hat{e}_R + E_\perp^* \hat{e}_L \right) / 2 \tag{2.1.46}
\]

The difference between these two irradiances is

\[
I_R - I_L = i \frac{k/2 \omega \mu_d}{(k/2 \omega \mu_d)^2} \left( E_\parallel^* \hat{e}_R - E_\parallel^* \hat{e}_L \right) \tag{2.1.47}
\]

Therefore the required Stokes parameters \( I, Q, U, V \) are

\[
I = \frac{k/2 \omega \mu_d}{(k/2 \omega \mu_d)^2} \left( E_\parallel^* E_\parallel + E_\perp^* E_\perp \right) \tag{2.1.48}
\]

\[
Q = \frac{k/2 \omega \mu_d}{(k/2 \omega \mu_d)^2} \left( E_\parallel^* E_\parallel - E_\perp^* E_\perp \right) \tag{2.1.49}
\]
Now, in case of scattering of the incident field by a particle the time averaged Poynting vector $\mathbf{S}$ at any point in the medium surrounding the particle can be written as the sum of three terms.

\[
\mathbf{S} = (1/2) \Re (\mathbf{E} \times \mathbf{H}^*) + \mathbf{S}_i + \mathbf{S}_s + \mathbf{S}_{ext}
\]

where,

\[
\mathbf{S}_i = (1/2) \Re (\mathbf{E}_i \times \mathbf{H}_i^*)
\]

\[
\mathbf{S}_s = (1/2) \Re (\mathbf{E}_s \times \mathbf{H}_s^*)
\]

\[
\mathbf{S}_{ext} = (1/2) \Re (\mathbf{E}_s \times \mathbf{H}_s^* \cdot \mathbf{E}_s \times \mathbf{H}_s^*)
\]

where $\mathbf{S}_i$ is the Poynting vector associated with the incident wave and is independent of position if the medium is nonabsorbing. $\mathbf{S}_s$ is the poynting vector of the scattered field and $\mathbf{S}_{ext}$ is the poynting vector arising because of interaction between the incident and scattered waves. If a suitably collimated detector of detector area $\Delta A$ is placed at a distance $r$ from the particle in the far field region, with $\Delta A$ aligned normal to $\hat{e}_t$, and if $\hat{e}_t$ is not too near the forward direction $\hat{e}_t (\theta = 0^\circ)$, the detector will record a signal proportional to

\[
\mathbf{S}_s \cdot \hat{e}_t, \Delta A
\]

provided $\Delta A$ is sufficiently small so that $\mathbf{S}_s$ does not vary greatly over the detector.

From 2.1.22 and 2.1.53 to 2.1.55 it follows that

\[
\mathbf{S}_s \cdot \hat{e}_t, \Delta A = \frac{k}{2\omega \mu_0} \frac{|A|^2}{k^2} \Delta \Omega
\]
where

\[ \Delta \Omega = \frac{A A}{r^2} \quad \text{2.1.58} \]

is the solid angle subtended by the detector. Hence it is possible to obtain \(|A|^2\) as a function of direction, to within a solid angle \(\Delta \Omega\) by recording the detector response at various positions on a hemisphere surrounding the particle. By interposing various polarizers in front of the detector and proceeding in a manner identical to the method used in finding relations 2.1.48 to 2.1.51, the Stokes parameters of the light scattered by a particle is obtained as

\[
I_s = \frac{k}{2} \alpha \mu (E_{||}E_{||}^* + E_{\perp}E_{\perp}^*) \\
Q_s = \frac{k}{2} \alpha \mu (E_{||}E_{||}^* - E_{\perp}E_{\perp}^*) \\
U_s = \frac{k}{2} \alpha \mu (E_{||}E_{\perp}^* + E_{\perp}E_{||}^*) \\
V_s = i \frac{k}{2} \alpha \mu (E_{||}E_{\perp}^* - E_{\perp}E_{||}^*)
\]

Thus relations 2.1.27, 2.1.48-2.1.51 and 2.1.59-2.1.62 yields

\[
\begin{pmatrix}
I_s \\
Q_s \\
U_s \\
V_s
\end{pmatrix} = \frac{1}{k^2 r^2} \begin{pmatrix}
S_{11} & S_{12} & S_{13} & S_{14} \\
S_{21} & S_{22} & S_{23} & S_{24} \\
S_{31} & S_{32} & S_{33} & S_{34} \\
S_{41} & S_{42} & S_{43} & S_{44}
\end{pmatrix} \begin{pmatrix}
I_t \\
Q_t \\
U_t \\
V_t
\end{pmatrix}
\]

where

\[
S_{11} = (1/2)(|S_1|^2 + |S_2|^2 + |S_3|^2 + |S_4|^2) \\
S_{12} = (1/2)(|S_2|^2 - |S_1|^2 + |S_4|^2 - |S_3|^2) \\
S_{13} = \text{Re}(S_2 S_3^* + S_1 S_4^*) \\
S_{14} = \text{Im}(S_2 S_3^* - S_1 S_4^*) \\
S_{21} = (1/2)(|S_2|^2 - |S_1|^2 - |S_4|^2 + |S_3|^2)
\]
Thus the 4×4 matrix in 2.1.63 is the required scattering matrix and is the Mueller matrix for scattering by a single particle. The element $S_{11}$ is related to the measurements made by the air quality monitoring system, a fact that becomes evident when 2.1.63 is used in developing the Mie theory.

2.2. Theory of extinction
Suppose that one or more particles are placed in a beam of electromagnetic radiation and the rate at which electromagnetic energy is received by a detector \( D \) downstream from the particles is denoted by \( U \). If the particles are removed, the power received by the detector is \( U_0 \), where \( U_0 > U \). Thus the presence of the particles results in extinction of the incident beam. If the medium in which the particles are embedded is nonabsorbing, the difference \( U_0 - U \) is accounted for by absorption in the particles and scattering by the particles.

To investigate extinction by a single arbitrary particle embedded in a non-absorbing medium and illuminated by a plane wave an imaginary sphere of radius \( r \) is constructed around the particle as in figure 2.4. Then the net rate \( W_a \) at which electromagnetic energy crosses the surface \( A_{sph} \) of this sphere is

\[
W_a = - \int_{A_{sph}} S \hat{e}_r dA \tag{2.2.1}
\]

where \( S \) is the Poynting vector. If \( W_a > 0 \), energy is absorbed within the sphere. But the medium is non-absorbing, which implies that \( W_a \) is the rate at which energy is absorbed by the particle. Because of the Stoke’s parameters 2.1.48-2.1.51 and Poynting vectors 2.1.53-2.1.55, \( W_a \) may be written as the sum of three terms

\[
W_i = - \int_{A_{sph}} S_i \hat{e}_r dA \tag{2.2.2}
\]

\[
W_s = \int_{A_{sph}} S_s \hat{e}_r dA \tag{2.2.3}
\]

and

\[
W_{ext} = - \int_{A_{sph}} S_{ext} \hat{e}_r dA \tag{2.2.4}
\]
Now, $W_i$ vanishes identically for a non-absorbing medium and $W_s$ is the rate at which energy is scattered across the surface $A_{\text{ph}}$. Therefore $W_{\text{ext}}$ is just the sum of the energy absorption rate and the energy scattering rate. Thus,

$$W_{\text{ext}} = W_a + W_s \quad \text{2.2.5}$$

For convenience the incident electric field $E_i = E\hat{e}_x$ is taken to be $x$-polarized. Because the medium is non-absorbing, $W_a$ is independent of the radius $r$ of the imaginary sphere. Therefore $r$ may be chosen sufficiently large such that it is in the far-field region where

$$E_s \sim \frac{e^{ik(r-r')}}{ikr} XE \quad \text{2.2.6}$$

$$H_s \sim \frac{k}{\omega \mu} \hat{e}_r \times E_s \quad \text{2.2.7}$$

and $\hat{e}_r \cdot X = 0$. As a reminder that the incident light is $x$-polarized the symbol $X$ is used for the vector scattering amplitude. The limiting values of $W_{\text{ext}}$ as $kr \rightarrow \infty$ is therefore [10]

$$W_{\text{ext}} = I_i \left(4\pi k^2\right) \Re\{X\hat{e}_x\theta_0\} \quad \text{2.2.8}$$

where $I_i$ is the incident irradiance. Now $C_{\text{ext}}$, defined as the cross-section of extinction, with dimensions of area, then becomes

$$C_{\text{ext}} = \frac{W_{\text{ext}}}{I_i} = \left(4\pi k^2\right) \Re\{X\hat{e}_x\theta_0\} \quad \text{2.2.9}$$

It follows from 2.2.5 that the $C_{\text{ext}}$ may be written as the sum of $C_{\text{abs}}$, the cross-section of absorption, and $C_{\text{sca}}$, the cross-section of scattering. Hence,

$$C_{\text{ext}} = C_{\text{abs}} + C_{\text{sca}} \quad \text{2.2.10}$$

where
\[ C_{abs} = \frac{W_{abs}}{I_i} \quad 2.2.11 \]

and

\[ C_{sca} = \frac{W_s}{I_i} \quad 2.2.12 \]

From 2.2.2-2.2.4 and 2.2.6-2.2.7 we have,

\[
C_{sca} = \frac{2\pi}{\kappa^2} \int_0^\infty \frac{|X|^2}{r^2} \sin \theta \, d\theta \, d\phi = \frac{1}{4\pi} \int \frac{|X|^2}{k^2} \, d\Omega \quad 2.2.13
\]

The quantity \( |X|^2 / k^2 \) is the differential scattering cross-section and \( dC_{sca}/d\Omega \) physically specifies the angular distribution of the scattered light, that is, the amount of light for unit incident irradiance scattered into a unit solid angle about a given direction. Now if \( N \) is the number of particles per unit volume of the medium through which extinction of light is taking place then the irradiance is attenuated according to the expression (2.1.10), which can be represented using 2.2.10-2.2.13 also as

\[ I = I_0 e^{-\sigma} \quad 2.2.14 \]

where

\[ \sigma = NC_{ext} = NC_{abs} + NC_{sca} \quad 2.2.15 \]

is the extinction co-efficient. The extinction co-efficient for a mixture of different particles may be represented as

\[ \sigma = \sum_j N_j C_{ext,j} \quad 2.2.16 \]

where \( N_j \) is the number of particles of type \( j \) per unit volume and \( C_{ext,j} \) is the corresponding extinction cross-section. The transmissiometer part of the air quality monitoring system is used to measure this extinction coefficient.
2.3. Mie theory

In order to investigate water vapour in the air, Mie theory\(^\text{[27,10,44]}\) is appropriate as it has been applied successfully to explain extinction and scattering by spherical particles and water vapour falls in this category of spherical particles at the detectable levels. Rayleigh and Raman scattering are left out as the particles being investigated are neither very small or has the appropriate density to be able to produce detectable levels of light flux. As it is known, Mie theory begins by expanding the incident plane \(x\)-polarized wave

\[
E_i = E_0 e^{i(kz-\omega t)} \hat{\varepsilon}_x
\]

written in spherical polar co-ordinates as

\[
E_i = E_0 e^{ik\cos \theta} \hat{\varepsilon}_x
\]

where

\[
\hat{\varepsilon}_x = \sin \theta \cos \phi \hat{\varepsilon}_r + \cos \theta \cos \phi \hat{\varepsilon}_\theta - \sin \phi \hat{\varepsilon}_\phi
\]

in vector spherical harmonics as,

\[
E_i = \sum_{m=0}^{\infty} \sum_{n=0}^{m} \left( B_{am} M_{am} + B_{cm} M_{cm} + A_{am} N_{am} + A_{cm} N_{cm} \right)
\]

with the vector spherical harmonics being given by the relations,

\[
M_{am} = -\frac{m}{\sin \theta} \sin m\phi P_n^m (\cos \theta) z_n(\rho) \hat{\varepsilon}_\theta - \cos m\phi \frac{dP_n^m (\cos \theta)}{d\theta} z_n(\rho) \hat{\varepsilon}_\phi
\]

\[
M_{cm} = \frac{m}{\sin \theta} \cos m\phi P_n^m (\cos \theta) z_n(\rho) \hat{\varepsilon}_\theta - \sin m\phi \frac{dP_n^m (\cos \theta)}{d\theta} z_n(\rho) \hat{\varepsilon}_\phi
\]
2.3.5

\[ N_{m\alpha n} = \frac{z_n(\rho)}{\rho} \cos m\phi n(n + 1)P_n^m(\cos \theta) \hat{e}_r, \]

\[ + \cos m\phi \frac{dP_n^m(\cos \theta)}{d\theta} \frac{1}{\rho} \frac{d}{d\rho} [\rho z_n(\rho)] \hat{e}_\theta \]

\[ - m \sin m\phi \frac{P_n^m(\cos \theta)}{\sin \theta} \frac{1}{\rho} \frac{d}{d\rho} [\rho z_n(\rho)] \hat{e}_\phi \]

2.3.6

\[ N_{m\alpha n} = \frac{z_n(\rho)}{\rho} \sin m\phi n(n + 1)P_n^m(\cos \theta) \hat{e}_r, \]

\[ + \sin m\phi \frac{dP_n^m(\cos \theta)}{d\theta} \frac{1}{\rho} \frac{d}{d\rho} [\rho z_n(\rho)] \hat{e}_\theta \]

\[ + m \cos m\phi \frac{P_n^m(\cos \theta)}{\sin \theta} \frac{1}{\rho} \frac{d}{d\rho} [\rho z_n(\rho)] \hat{e}_\phi \]

2.3.7

where \( P_n^m \) are the Associated Legendre Polynomials of degree \( n \) and order \( m \),

\( z_n \) is a Bessel function,

\( \rho = kr, k \) being the propagation constant, is a dimensionless parameter and

\( B_{m\alpha n}, B_{\alpha m n}, A_{m\alpha n}, A_{\alpha m n} \) are the expansion co-efficients.

The orthogonality of all the vector spherical harmonics implies that the expansion co-efficients in 2.3.3 are of the form

\[ B_{m\alpha n} = \frac{\int_0^{2\pi} \int_0^\pi E_\lambda M_{m\alpha n} \sin \theta d\theta d\phi}{\int_0^{2\pi} \int_0^\pi |M_{m\alpha n}|^2 \sin \theta d\theta d\phi} \]
with similar expressions for \( B_{\text{omm}} \), \( A_{\text{emm}} \) and \( A_{\text{onn}} \). It follows from 2.3.2, 2.3.4 and 2.3.7 together with the orthogonality of sine and cosine that \( B_{\text{emm}} = A_{\text{onn}} = 0 \) for all \( m \) and \( n \).

Moreover, the remaining co-efficients vanish unless \( m=1 \) for the same reason.

The expansion co-efficients that finally remain after evaluation are

\[
B_{\text{eln}} = i^n E_0 \frac{2n + 1}{n(n + 1)} \quad 2.3.8
\]

and

\[
A_{\text{eln}} = -iE_0 i^n \frac{2n + 1}{n(n + 1)} \quad 2.3.9
\]

Now since the incident field is finite at the origin it is required that, from the two spherical Bessel functions [3]

\[
j_n(\rho) = \sqrt{\frac{\pi}{2\rho}} J_{n+\frac{1}{2}}(\rho) \quad 2.3.10
\]

and

\[
y_n(\rho) = \sqrt{\frac{\pi}{2\rho}} Y_{n+\frac{1}{2}}(\rho) \quad 2.3.11
\]

where \( J_\nu \) ans \( Y_\nu \) are the Bessel functions of first and second kind, \( z_n \) in the vector spherical harmonics be the spherical Bessel funtion \( j_n(\rho) \) as it is well behaved at the origin. Since the spherical Bessel function satisfy the recurrence relations

\[
z_{n-1}(\rho) + z_{n+1}(\rho) = \frac{2n + 1}{\rho} z_n(\rho) \quad 2.3.12
\]

and

\[
(2n + 1) \frac{d}{d\rho} z_n(\rho) = nz_{n-1}(\rho) - (n + 1)z_{n+1}(\rho) \quad 2.3.13
\]

from the first two orders,

\[
j_0(\rho) = (\sin \rho)/\rho \quad \text{and} \quad j_1(\rho) = \sin \rho/\rho^2 - \cos \rho/\rho,
\]
higher order terms can be generated. Hence the superscript (1) is appended to vector spherical harmonics involving \( j_n(\rho) \). The expansion of the plane wave in spherical harmonics finally takes the form

\[
E_i = E_0 \sum_{n=1}^{\infty} i^n \frac{2n+1}{n(n+1)} (M_{oln}^{(1)} - iN_{eln}^{(1)})
\]

and the corresponding incident magnetic field is obtained from the curl of 2.3.14 as

\[
H_i = -\frac{k}{\omega \mu} E_0 \sum_{n=1}^{\infty} i^n \frac{2n+1}{n(n+1)} (M_{eln}^{(0)} + iN_{oln}^{(0)})
\]

When the plane \( x \)-polarized wave is incident on a homogeneous, isotropic sphere of radius \( a \), the fields inside the particle are given as

\[
E_1 = \sum_{n=1}^{\infty} E_n (c_n M_{oln}^{(0)} - id_n N_{eln}^{(0)})
\]

and

\[
H_1 = -\frac{k}{\omega \mu} \sum_{n=1}^{\infty} E_n (d_n M_{eln}^{(0)} + ic_n N_{oln}^{(0)})
\]

where \( E_n = i^n E_0 \frac{(2n+1)}{n(n+1)} \), \( \mu_l \) is the permeability of the sphere and \( c_n \) and \( d_n \) are the expansion co-efficients.

In case of the scattered field the expressions arrived at are

\[
E_s = \sum_{n=1}^{\infty} E_n (ia_n N_{aeln}^{(3)} + b_n M_{oln}^{(3)})
\]

and

\[
H_s = \frac{k}{\omega \mu} \sum_{n=1}^{\infty} E_n (i b_n N_{oln}^{(2)} + a_n M_{aeln}^{(2)})
\]
where \( a_n \) and \( b_n \) are the expansion co-efficients and the superscript \( (2) \) appended to the vector spherical harmonics indicate that the Bessel function \( z_n \) in these harmonics is the spherical Hankel function

\[
h_n(kr) \sim \frac{(-i)e^{ikr}}{ikr} \quad kr>>n^2
\]  

For simplifying the vector spherical harmonics it is found to be convenient to define two functions

\[
\pi_n = \frac{P_n}{\sin \theta}
\]  

and \[
\tau_n = \frac{d}{d\theta} P_n
\]  

which can be computed by beginning with \( \pi_0=0 \) and \( \pi_1=1 \) since they follow the recurrence relations

\[
\pi_n = \frac{2n-1}{n-1} \mu \pi_{n-1} - \frac{n}{n-1} \pi_{n-2}
\]  

\[
\tau_n = n \mu \pi_n - (n+1) \pi_{n-1}
\]  

where \( \mu = \cos \theta \)

\[
\pi_n(-\mu) = (-1)^{n-1} \pi_n(\mu)
\]  

\[
\tau_n(-\mu) = (-1)^n \tau_n(\mu)
\]  

and \( \pi_n + \tau_n \) and \( \pi_n - \tau_n \) are orthogonal

The vector spherical harmonics 2.3.4 - 2.3.7 with \( m=1 \) in the expansions of the internal fields 2.3.16 and 2.3.17 and the scattered fields 2.3.18 and 2.3.19 can now be written in a more concise form as
\[ \mathbf{M}_{\text{eln}} = \cos \phi \pi_n(\cos \theta)z_n(\rho)\hat{\rho} - \sin \phi \tau_n(\cos \theta)z_n(\rho)\hat{\phi} \]

2.3.29

\[ \mathbf{M}_{\text{eln}} = -\sin \phi \pi_n(\cos \theta)z_n(\rho)\hat{\theta} - \cos \phi \tau_n(\cos \theta)z_n(\rho)\hat{\phi} \]

2.3.30

\[ \mathbf{N}_{\text{eln}} = \sin \phi n(n+1)\sin \theta \pi_n(\cos \theta)\frac{z_n(\rho)}{\rho} \hat{r} + \sin \phi \tau_n(\cos \theta)\frac{[\rho z_n(\rho)]'}{\rho} \hat{\theta} + \cos \phi \pi_n(\cos \theta)\frac{[\rho z_n(\rho)]'}{\rho} \hat{\phi} \]

2.3.31

\[ \mathbf{N}_{\text{eln}} = \cos \phi n(n+1)\sin \theta \pi_n(\cos \theta)\frac{z_n(\rho)}{\rho} \hat{r} + \cos \phi \tau_n(\cos \theta)\frac{[\rho z_n(\rho)]'}{\rho} \hat{\theta} - \sin \phi \pi_n(\cos \theta)\frac{[\rho z_n(\rho)]'}{\rho} \hat{\phi} \]

2.3.32

where the prime indicates differentiation, a process that is aided by the identity

\[ \frac{d}{d\rho} z_n = \frac{n z_{n-1} - (n+1)z_{n+1}}{2n+1} \]

2.3.33

Now the boundary conditions at the boundary between the spherical particle and the medium are given as

\[ (E_i + E_s - E_j) \times \hat{r} = 0 \]

2.3.34

\[ (H_i + H_s - H_j) \times \hat{r} = 0 \]

2.3.35

and may be written in component form as

\[ E_{i\theta} + E_{s\theta} = E_{i\theta} \]

2.3.36

\[ E_{i\phi} + E_{s\phi} = E_{i\phi} \]

2.3.37
\[ H_{i\theta} + H_{s\theta} = H_{1\theta} \quad 2.3.38 \]

\[ H_{i\phi} + H_{s\phi} = H_{1\phi} \quad 2.3.39 \]

Hence from the orthogonality of \( \sin \phi \) and \( \cos \phi \), the orthogonality relations 2.3.28, the boundary conditions 2.3.36-2.3.39, the expansions 2.3.14-2.3.19 and the expressions 2.3.29-2.3.32 for the vector spherical harmonics, four linear equations are eventually obtained in the expansion coefficients as

\[ j_n(mx)c_n + h_n(x)b_n = j_n(x) \quad 2.3.40 \]

\[ \mu[mxj_n(mx)]'c_n + \mu_1[xh_n(x)]'b_n = \mu_1[xj_n(x)]' \quad 2.3.41 \]

\[ \mu mj_n(mx)d_n + \mu_1h_n(x)a_n = \mu_1j_n(x) \quad 2.3.42 \]

\[ [mxj_n(mx)]'d_n + m[xh_n(x)]'a_n = m[xj_n(x)]' \quad 2.3.43 \]

where the prime indicates differentiation with respect to the argument in parenthesis and the size parameter \( x \) and the relative refractive index \( m \) are

\[ x = \frac{ka}{\lambda} = \frac{2\pi Na}{\lambda} \quad 2.3.44 \]

\[ m = \frac{k_1}{k} = \frac{N_1}{N} \quad 2.3.45 \]

and \( N_1 \) and \( N \) are the refractive indices of particle and medium, respectively. Solving the four simultaneous equations 2.3.40 - 2.3.43, the scattering coefficients are obtained as

\[ a_n = \frac{\mu m^2 j_n(mx)[xj_n(x)]' - \mu_1 j_n(x)[mxj_n(mx)]'}{\mu m^2 j_n(mx)[xh_n(x)]' - \mu_1 h_n(x)[mxj_n(mx)]'} \quad 2.3.46 \]

\[ b_n = \frac{\mu_1 j_n(mx)[xj_n(x)]' - \mu j_n(x)[mxj_n(mx)]'}{\mu_1 j_n(mx)[xh_n(x)]' - \mu h_n(x)[mxj_n(mx)]'} \quad 2.3.47 \]
These coefficients are further simplified by introducing the Riccati-Bessel functions [27]

\[
\psi_n(p) = \rho j_n(p) \tag{2.3.48}
\]

and \[
\xi_n(p) = \rho h_n(p) \tag{2.3.49}
\]

with \( \xi_n \) also represented as,

\[
\xi_n = \psi_n - i\chi_n \tag{2.3.50}
\]

where \( \chi_n(p) = -\rho y_n(p) \) is a Ricatti-Bessel function with \( y_n \) given by 2.3.11. If the permeability \( \mu \) and \( \mu \) of the particle and the surrounding medium, respectively, is the same, then 2.3.46 and 2.3.47 become

\[
a_n = \frac{m\psi_n(mx)\psi'_n(x) - \psi_n(x)\psi'_n(mx)}{m\psi_n(mx)\xi'_n(x) - \xi_n(x)\psi'_n(mx)} \tag{2.3.51}
\]

\[
b_n = \frac{\psi_n(mx)\psi'_n(x) - m\psi_n(x)\psi'_n(mx)}{\psi_n(mx)\xi'_n(x) - m\xi_n(x)\psi'_n(mx)} \tag{2.3.52}
\]

Since the series expansion 2.3.18 and 2.3.19 of the scattered field is uniformly convergent, the series can be terminated after \( n_c \) terms and the resulting error is arbitrarily small for all \( kr \) if \( n_c \) is sufficiently large. Now if \( kr \gg n_c^2 \), substituting the asymptotic relation 2.3.20 and its derivative,

\[
\frac{dh_n}{dp} \sim \frac{(-i)^n e^{ip}}{\rho} \tag{2.3.53}
\]

which is obtained by using the identity 2.3.33, in the truncated series of 2.3.18 and 2.3.19, yields the transverse components of the scattered electric field as

\[
E_{se} \sim E_0 \frac{e^{i\varphi}}{-ikr} \cos \phi \ S_x (\cos \theta) \tag{2.3.54}
\]
and \( E_{s \phi} \sim -E_0 e^{i \alpha r} \sin \phi \ S_1 (\cos \theta) \) \quad 2.3.55

where,
\[
S_1 = \sum_n \frac{2n + 1}{n(n + 1)} (a_n r_n + b_n r_n)
\]
\[
S_2 = \sum_n \frac{2n + 1}{n(n + 1)} (a_n r_n + b_n r_n)
\]

and the series are terminated after \( n_c \) terms. The relation between incident and scattered field amplitudes therefore becomes
\[
\begin{pmatrix}
E_{1s} \\
E_{2s}
\end{pmatrix} = \frac{e^{ikr}}{-ikr} \begin{pmatrix}
S_2 & 0 \\
0 & S_1
\end{pmatrix} \begin{pmatrix}
E_{1i} \\
E_{2i}
\end{pmatrix}
\]

From this relation 2.3.58 and using the 4x4 Mueller matrix for scattering from 2.1.63, the relation between incident and scattered Stokes parameters follows as
\[
\begin{pmatrix}
I_s \\
Q_s \\
U_s \\
V_s
\end{pmatrix} = \frac{1}{k^2 r^2} \begin{pmatrix}
S_{11} & S_{12} & 0 & 0 \\
S_{12} & S_{11} & 0 & 0 \\
0 & 0 & S_{33} & S_{34} \\
0 & 0 & -S_{34} & S_{33}
\end{pmatrix} \begin{pmatrix}
I_i \\
Q_i \\
U_i \\
V_i
\end{pmatrix}
\]

where,
\[
S_{11} = \frac{1}{2} (|S_2|^2 + |S_1|^2)
\]
\[
S_{12} = \frac{1}{2} (|S_2|^2 - |S_1|^2)
\]
\[
S_{33} = \frac{1}{2} (S_2^* S_1 + S_2 S_1^*)
\]
\[
S_{34} = \frac{i}{2} (S_1 S_2^* - S_2 S_1^*)
\]
If the incident light is unpolarized then due to relations 2.1.59 – 2.1.62 the Stoke's parameters of the scattered light in 2.3.59 become

\[ U_t = V_t = 0 \]  
\[ Q_s = (1/k^2 \ell^2) S_{12} I, \]  
\[ I_s = (1/k^2 \ell^2) S_{11} I, \]

Since the Stokes parameters of the light scattered by a collection of randomly separated particles are the sum of the Stokes parameters of the light scattered by the individual particles, therefore the scattering matrix for such a collection is merely the sum of the individual particle scattering matrices, provided linear dimension of the volume occupied by the scatterers is small compared with the distance \( r \) at which the scattered light is observed. Following the theory of self preserving size distribution [39,9,58,71,32] which suggests that in a unit volume of natural aerosols the sizes of the particles is given by a distribution function [11,61,35,8,14,13,56] the distribution used for the air quality monitoring system is the gamma distribution [39] given by

\[ N(a) = p a^\gamma e^{-\eta a} \]

where \( a \) is the radius of the particle and \( p, \gamma, \eta \) are parameters of the distribution related to the density of scattering particles \( N_{\text{tot}} \) by

\[ N_{\text{tot}} = p \eta^{-\gamma(\gamma+1)} \Gamma(\gamma+1) \]

where again \( \gamma \) and \( \eta \) are related to the particle radius \( a_c \) corresponding to the peak of the distribution, the so-called modal radius, by

\[ a_c = \gamma/\eta \]

Hence, if the particle density \( N_{\text{tot}} \) is fixed, the gamma distribution 2.3.67 is completely specified by the index \( \gamma \) and the modal radius \( a_c \). Therefore, for all calculations the
standard density of $N_{\text{tot}} = 100 \, \text{cm}^{-3}$ is assumed and integrals over $N(a)$ are normalized to this density. For $\gamma$ a range of values 1 to 4 and for $a_c$ a range of values 0.1 – 10 $\mu$m are assumed as these parameter values are appropriate to the water vapour conditions during experiments with the air quality monitoring system.

The use of size distribution then leads to the formation of the volume scattering coefficient $\beta(\theta)$ for unpolarized light [7,63,24,38] which is obtained by integrating $S_{\text{II}}$ as given by 2.3.66 over the size distribution $N(a)$ and is given as,

$$
\beta(\theta) = \frac{1}{k^3} \int_0^\infty N(a)S_{\text{II}}(\theta)da \quad 2.3.70
$$

where $\beta(\theta)$ is in units of per steradian per centimeter ($\text{sr}^{-1}\text{cm}^{-1}$).

Thus it is evident from 2.3.66 and 2.3.70 that experimental measurements of $I_r$ and $I_i$ using unpolarized light will yield experimental $\beta(\theta)$ values, a fact that is very much used in the air quality monitoring system.

2.4 Computation of Scattering coefficients.

For a particular scattering angle $\theta$, assuming some initial values for $\alpha, \lambda, N$ and $N_I$ in 2.3.44 and 2.3.45 and then using relations 2.3.23, 2.3.24, 2.3.51 and 2.3.52 the values of $\pi_n, \tau_n, \alpha_n$ and $b_n$ may be derived and put in 2.3.56 and 2.3.57 to obtain the values of $S_I$ and $S_2$ which when put in 2.3.60 gives the value of $S_{\text{II}}$ for the particular $\theta$. Similarly deriving the values of $S_{\text{II}}$ for a range of particle radii $a$ and using 2.3.67 the corresponding value of $\beta(\theta)$ can be derived. This aspect of the theory is taken advantage of in developing a software to simulate, using dummy initial values, theoretical results of $\beta(\theta)$ over a wide range of size distributions $N(a)$ and over a range of angles $\theta$ which may be used in drawing a co-relation with the experimental
results obtained when the air quality monitoring system is working as a nephelometer.

In computation of scattering coefficients [10] the logarithmic derivative

\[ D_n(\rho) = \frac{d}{d\rho} \log_e \psi_n(\rho) \]  \hspace{1cm} 2.4.1

which as a consequence of relations 2.3.12 and 2.3.13 satisfies the recurrence relation

\[ D_{n-1} = \frac{n}{\rho} - \frac{1}{\rho} D_n + \frac{n}{\rho} \]  \hspace{1cm} 2.4.2

is introduced, as this recasts the equations 2.3.51 and 2.3.52 in a convenient form given as

\[ a_n = \frac{\left[ \frac{D_n(mx)}{m} + \frac{n}{x} \right] \psi_n(x) - \psi_{n-1}(x)}{\left[ \frac{D_n(mx)}{m} + \frac{n}{x} \right] \xi_n(x) - \xi_{n-1}(x)} \]  \hspace{1cm} 2.4.3

\[ b_n = \frac{\left[ mD_n(mx) + \frac{n}{x} \right] \psi_n(x) - \psi_{n-1}(x)}{\left[ mD_n(mx) + \frac{n}{x} \right] \xi_n(x) - \xi_{n-1}(x)} \]  \hspace{1cm} 2.4.4

where the recurrence relations

\[ \psi'_n(x) = \psi_{n-1}(x) - \frac{n\psi_n(x)}{x} \]  \hspace{1cm} 2.4.5

\[ \xi'_n(x) = \xi_{n-1}(x) - \frac{n\xi_n(x)}{x} \]  \hspace{1cm} 2.4.6

are used to eliminate \( \psi' \) and \( \xi' \). In the computations, \( D_n(mx) \) in 2.4.1 is calculated using 2.4.2 by downward recurrence [10], that is lower orders are calculated from higher orders. Again \( \psi_n(x) \) and \( \xi_n(x) \), which are given by 2.3.48 and 2.3.50, are
calculated by upward recurrence, that is higher orders are calculated from lower orders using 2.3.12 and 2.3.13. This ensures stability in the calculations of \( D_n(mx) \), \( \psi_n(x) \) and \( \xi_n(x) \) as they are related to the stability in the calculations of the spherical Bessel functions \( j_n \) and \( y_n \) using their recurrence relations.

The C language [62,74] program "miescat.c" has been developed for the designed air quality monitoring system to compute theoretical values of \( S_{11} \) and the subsequent values of \( \beta \) as a part of this doctoral work. The program thus developed borrows ideas from the FORTRAN program of Bohren and Huffman [10] who in turn developed it from Dave's program [37]. But in its totality, the "miescat.c" thus developed is sufficiently different from that program. The chief difference between these two programs are that while Bohren and Huffman's program deals with scattering by a single particle, our program deals with scattering from multiple particles incorporated in the relevant equation through the size distribution function.

In the program the approximate number of terms \( NSTOP \) required for convergence of 2.3.51 and 2.3.52 and consequently 2.4.3 and 2.4.4 is given by the integer closest to [73],

\[
x + 4x^{1/3} + 2
\]

Again \( D_n(mx) \) is computed by downward recurrence beginning with \( D_{MAX} = 0.0 + 0.0i \) where \( NMX \) is taken to be the value obtained by adding 15 with the greater of the two numbers \( NSTOP \) and \( |mx| \), that is, \( \text{Max}(NSTOP, |mx|) + 15 \). Both \( \psi_n \) and \( \xi_n \) are computed by upward recurrence beginning with

\[
\psi_{-1}(x) = \cos x
\]

\[
\psi_0(x) = \sin x
\]
\[ \chi_J(x) = -\sin x \]
\[ \chi_0(x) = \cos x \]

The angle-dependent functions \( \pi_n \) and \( \tau_n \) are computed using upward recurrence relations 2.3.23 and 2.3.24. The \( S_{II} \) values and consequently the \( \beta(\theta) \) values for angles from 22.5° to 157.5° in steps of 4.5° are computed for a given size distribution with the modal radius \( a_c \) being given as input and then these values are normalized with respect to the value of \( \beta(22.5^\circ) \). The outputs of the program are stored in memory so that they can be tallied with the experimental results later.

The flowchart for the program "miescat.c" is given below in figure 2.5a-2.5d.
Figure 2.5a Flowchart of "miescat.c" program for computation of volume scattering coefficient by spherical water droplets of different size distributions

start

refractive index of particle \( N_i = 1.33 + i \times 10^{-8} \)
refractive index of medium \( N = 1.00 + i 0.0 \)
wavelength of laser source \( \lambda = 0.6328\mu m \)

\[ m = \frac{N_i}{N} \]

enter filename for storage of results,
enter the modal radius \( a_c \)

\[ \theta = 0.0 \]

\[ \beta_{\text{tot}}(\theta) = 0.0 \]

\[ \theta = \theta + 4.5^\circ \]

is \( \theta = 180^\circ \)?

No

radius \( a = 0.1 \mu m \)

\[ x = 2\pi aN/\lambda \]

\[ \gamma = 2; \ n_{\text{tot}} = 100 \]

\[ \eta = \gamma/a_c \]
\[ \Gamma(\gamma + 1) = \gamma! \]

\[ p = n_{\text{tot}}/\{\eta^{(\gamma+1)}\Gamma(\gamma+1)\} \]

\[ n(a) = pa^{7}e^{-7} \]

\[ \beta_{\text{normal}}(\theta) = \beta_{\text{tot}}(\theta)/\beta_{\text{tot}}(22.5^\circ) \]

\[ \theta = 22.5^\circ \]

is \( \theta = 157.5^\circ \)?

No

\[ \theta = \theta + 4.5^\circ \]

record \( \theta \) and \( \beta_{\text{normal}}(\theta) \) in file

\[ a = a + 0.2\mu m \]

No

\[ a = 30.0\mu m \]

Yes

is \( \theta = 180^\circ \)?

No

\[ \theta = \theta + 4.5^\circ \]

\[ \beta_{\text{tot}}(\theta) = \beta_{\text{tot}}(\theta) + S_{11}(\theta) \times n(a) \times 0.2\mu m \]

\[ S_{11}(\theta) = \frac{1}{2}(|S_2(\theta)|^2 + |S_1(\theta)|^2) \]

\[ \theta = 0.0^\circ \]

call subroutine BH MIE and return

end
Figure 2.5b Flowchart of "miescat.c" (continued)
\[ \psi_1 = \cos(x) \quad \psi_0 = \sin(x) \quad \chi_1 = -\sin(x) \quad \chi_0 = \cos(x) \]

\[ \xi_0 = \psi_0 - i \chi_0 \]

\[ n = 1 \]

\[ \psi_1 = \frac{2n - 1}{x} \psi_0 - \psi_{-1} \]

\[ \chi_1 = \frac{2n - 1}{x} \chi_0 - \chi_{-1} \]

\[ \xi_i = \psi_i - i \chi_i \]

\[ a(n) = \frac{[D(n)/m + n/x] \psi_1 - \psi_0}{[D(n)/m + n/x] \xi_1 - \xi_0} \]

\[ b(n) = \frac{[mD(n) + n/x] \psi_1 - \psi_0}{[mD(n) + n/x] \xi_1 - \xi_0} \]

\[ \theta = 0.0^\circ \]

\[ \pi(\theta) = \pi_1(\theta) \]

\[ \tau(\theta) = n\mu(\theta)\pi(\theta) - (n+1)\kappa(\theta) \]

Figure 2.5c Flowchart of "miescat.c" (continued)
Figure 2.5d Flowchart of "miescat.c" (continued)
This C language program "miescat.c" is given below

```c
#include <stdio.h>
#include <math.h>
#include "cpxarith.c"
#define PI 3.14159265e+0

main()
{
    char filename[10];
    double nr, slltot[45], rc;
    struct complex refrelk, slk[200], s2k[200], refmed;
    double refre=1.33e+0, refim=1.0e-8, s11, \
    rad, wavel=0.6328e-6, xk, ang, dang, sllnor;
    int nangk=21, nan, j, aj;
    void bhmie();
    double nrf();
    FILE *fp;
    printf("filename =");
    scanf("%s",filename);
    fp = fopen(filename,"w");
    printf("modal radius =");
    scanf("%lf", &rc);
    refmed.x=1.0e+0;
    refmed.y=0.0e+0;
    refrelk.x=refre;
    refrelk.y=refim;
    refrelk=cpxdiv(refrelk,refmed);
    for(j=1;j<=45;j++)
    {
        slltot[j]=0.0;
    }
    for(rad=0.0e-6;rad<=0.30e-6;rad=rad+0.2e-6)
    {
        nr=nrf(rad,rc);
        xk=2.0e+0 * PI * rad * (refmed.x)/wavel;
        dang=(PI/2.0e+0)/(double)(nangk-1);
        bhmie(&xk,&refrelk,&nangk,slk,s2k);
        nan=2*nangk-1;
        for(j=1;j<=nan;j++)
        {
            aj=j;
            sll=0.5e+0*(pow(cabs(s2k[j]),2.0e+0)+pow(cabs(slk[j]),2.0e+0));
            ang=dang*(aj-1.0e+0)*(180.0e+0/PI);
            slltot[j]=slltot[j]+sll*nr*0.2e-6;
        }
    }
    for(j=6;j<=nan-5;j++)
    {
        ang=dang*((double)j-1.0e+0)*(180.0e+0/PI);
        fprintf(fp,"%e,%e,\n",ang,slltot[j]/slltot[6]);
    }
    fclose(fp);
    printf("done");
    return(0);
}
void bhmie(double *x, struct complex *refrel, int *nang, struct complex sl[1], \n```
struct complex s2[]
{
  double amu[100], theta[100], pi[100], tau[100], pi0[100], pil[100];
  struct complex
d[3000], y, xi, xil, an, bn, an1, an2, bn1, bn2, compl, comp2, comp3,
  comp4, comp5;
  double psi0, psi, psil, d, dx, xstop, nstop, ymod, dang, rn, chi, chi0,
  chil, apsi0, apsil, apsi, fn, p, t;
  int nn, n, nmax, j, jj;
  dx=*x;
  anl.x=*x;
  anl.y=0.0e+0;
  y=cpxmult(anl, *refrel);
  xstop=*x+4.0e+0*pow(*x, 0.333e+0)+2.0e+0;
  nstop=xstop;
  ymod=cabs(y);
  nmax=(int) (max(xstop, ymod)) + 15;
  dang=(PI/2.0e+0)/(double)(*nang-l);
  for(j=1; j <= *nang; j++)
  {
    theta[j]=((double)(j)-1.0e+0)*dang;
    amu[j]=cos(theta[j]);
  }
  d[nmax].x=0.0e+0;
  d[nmax].y=0.0e+0;
  im=nmax-l;
  for (n=l; rt<=nn; n=n+l)
  {
    rn=(double)(nmax-n+1);
    anl.x=rn;
    anl.y=0.0;
    an2.x=1.0e+0;
    an2.y=0.0e+0;
    d[nmax-n]=cpxsub(cpxdiv(anl, y), 
                    cpxdiv(an2, cpxadd(d[nmax-n+1], 
                        cpxdiv(an1, y))));
  }
  for(j=1; j <= *nang; j++)
  {
    pi0[j]=0.0;
    pil[j]=1.0;
  }
  nn=2**nang-l;
  for (j=1; j<=nn; j++)
  {
    s1[j].x=0.0;
    s1[j].y=0.0;
    s2[j].x=0.0;
    s2[j].y=0.0;
  }
p.si0 = cos(dx);
p.sil = sin(dx);
chi0 = -sin(*x);
chi1 = cos(*x);
apsi = psil;
xil.x = apsil;
xil.y = -chil;
n=1;
lab200:
dn=(double)(n);
\[ m = \text{double}(n) \]
\[ fn = \frac{2.0 \times m + 1.0}{m \times (r_{n+1})}; \]
\[ \psi = (2.0 \times d_{n} - 1.0) \frac{\psi_{\text{in}}}{dx} - \psi_{0}; \]
\[ \alpha_{\psi} = \psi; \]
\[ \chi = (2.0 \times m - 1.0) \frac{\chi_{\text{in}}}{(x)} - \chi_{0}; \]
\[ x_{i,x} = \alpha_{\psi}; \]
\[ x_{i,y} = -\chi; \]
\[ anl = \text{cpxdiv}(d[n], \text{refrel}); \]
\[ \text{compl}.x = r_{n} / (*x); \]
\[ \text{compl}.y = 0.0; \]
\[ \text{comp}2.x = \alpha_{\psi}; \]
\[ \text{comp}2.y = 0.0; \]
\[ \text{comp}3.x = \alpha_{\psi}; \]
\[ \text{comp}3.y = 0.0; \]
\[ anl = \text{cpxadd}(anl, \text{compl}); \]
\[ anl = \text{cpxmult}(anl, \text{comp}2); \]
\[ anl = \text{cpxsub}(anl, \text{comp}3); \]
\[ an2 = \text{cpxdiv}(d[n], \text{refrel}); \]
\[ an2 = \text{cpxadd}(an2, \text{comp}1); \]
\[ an2 = \text{cpxmult}(an2, x_{i}); \]
\[ an2 = \text{cpxsub}(an2, x_{i1}); \]
\[ an = \text{cpxdiv}(anl, an2); \]
\[ anl = \text{cpxmult}(anl, \text{corap2}); \]
\[ anl = \text{cpxsub}(anl, \text{corap3}); \]
\[ an2 = \text{cpxmult}(\text{corap1}, d[n]); \]
\[ an2 = \text{cpxadd}(an2, \text{comp}1); \]
\[ an2 = \text{cpxmult}(an2, x_{i}); \]
\[ an2 = \text{cpxsub}(an2, x_{i1}); \]
\[ bn = \text{cpxdiv}(anl, an2); \]
\[ \text{for}(j = 1; j <= \text{nang}; j++) \{
\]
\[ \text{jj} = 2^{\text{nang}} - j; \]
\[ \text{pi}[j] = \text{pi}[j]; \]
\[ \tau[j] = r_{n} * \text{amu}[j] * \text{pi}[j] - (r_{n} + 1.0e+0) * \text{pi0}[j]; \]
\[ p = \text{pow}(-1.0e+0, \text{double}(n-1)); \]
\[ \text{compl}.x = \text{pi}[j]; \]
\[ \text{compl}.y = 0.0e+0; \]
\[ \text{comp}2.x = \tau[j]; \]
\[ \text{comp}2.y = 0.0e+0; \]
\[ \text{comp}3.x = fn; \]
\[ \text{comp}3.y = 0.0e+0; \]
\[ anl = \text{cpxmult}(an, \text{compl}); \]
\[ an2 = \text{cpxmult}(bn, \text{comp}2); \]
\[ anl = \text{cpxmult}(\text{comp}3, \text{cpxadd}(an1, an2)); \]
\[ s1[j] = \text{cpxadd}(s1[j], an1); \]
\[ t = \text{pow}(-1.0e+0, \text{double}(n)); \]
\[ anl = \text{cpxmult}(an, \text{comp}2); \]
\[ an2 = \text{cpxmult}(bn, \text{comp}1); \]
\[ anl = \text{cpxmult}(\text{comp}3, \text{cpxadd}(an1, an2)); \]
\[ s2[j] = \text{cpxadd}(s2[j], an1); \]
\[ \text{if}(j = jj) \{
\]
\[ \text{compl}.x = \text{pi}[j]; \]
\[ \text{compl}.y = 0.0e+0; \]
\[ \text{comp}2.x = \tau[j]; \]
\[ \text{comp}2.y = 0.0e+0; \]
\[ \text{comp}3.x = fn; \]
\[ \text{comp}3.y = 0.0e+0; \]
\[ \text{comp}4.x = p; \]
comp4.y=0.0;  
comp5.x=t;  
comp5.y=0.0;  
s1[jj]=cpxadd(s1[jj],cpxmult(comp3,cpxadd(  
cpxmult(an,cpxmult(comp1,comp4)),  
cpxmult(bn,cpxmult(comp2,comp5)))));

s2[jj]=cpxadd(s2[jj],cpxmult(comp3,  
cpxadd(  
cpxmult(an,cpxmult(comp2,comp5),
  
cpxmult(bn,cpxmult(comp1,comp4)))));
}

psi0=psil;  
psil=psi;  
apsil=psil;  
chi0=chi;  
chil=chi;  
xil.x=apsil;  
xil.y=chil;  
n=n+1;

rn=(double)(n);

for(j=1; j<=nang; j++)
{
    pil[j] = (2.0*rn-l.0)/(rn-1.0)*amu[j]*pi[j];
    pil[j] = pil[j] - rn*pi0[j]/(rn-1.0);
    pi0[j] = pi[j];
}

if((n-l-nstop)<0)
    goto lab200;
return;

double nrf(double radi, double rcc)
{
    double l, alfa=4.0e+0, b, a, n=100.0e+0, nr, gama=1.0e+0;
    b=alfa/rcc;
    for(l=alfa; l>=1.0e+0; l=1-1.0e+0)
    {
        gama= gama+l;
        a=n/( pow(b,-(alfa+l.0))*gama);
        nr=a*pow(radi,alfa)*exp(-b*radi);
        return(nr);
    }
}

Also the header file "cpxarith.c" that is used in the above program to do the complex
number arithmetic is given below

cpxarith.c

#include<math.h>
#include<stdlib.h>
#include<stdio.h>

struct complex cpxadd(struct complex z, struct complex w)
{
    struct complex Z;
    Z.x=z.x+w.x;
    Z.y=z.y+w.y;
    return Z;
}
struct complex cpxsub(struct complex z, struct complex w)
{
    struct complex Z;
    Z.x=z.x-w.x;
    Z.y=z.y-w.y;
    return Z;
}

struct complex cpxmult(struct complex z, struct complex w)
{
    struct complex Z;
    Z.x=(z.x)*(w.x)-(z.y)*(w.y);
    Z.y=(z.y)*(w.x)+(z.x)*(w.y);
    return Z;
}

struct complex cpxdiv(struct complex n, struct complex d)
{
    struct complex Z;
    double temp1,temp2;
    if(cabs(d)<(5.0e-20)*cabs(n)){
        fprintf(stderr,"division by zero in cpxdiv");
        exit(1);
    }
    if(fabs(d.x)<=fabs(d.y)){
        temp1=d.x/d.y;
        temp2=d.y+temp1*d.x;
        Z.x=(temp1*n.x+n.y)/temp2;
        Z.y=(temp1*n.y-n.x)/temp2;
    }
    else{
        temp1=d.y/d.x;
        temp2=d.x+temp1*d.y;
        Z.x=(n.x+temp1*n.y)/temp2;
        Z.y=(n.y-temp1*n.x)/temp2;
    }
    return Z;
}

struct complex conjg(struct complex z)
{
    struct complex Z;
    Z.x=z.x;
    Z.y=-z.y;
    return Z;
}

The program "miescat.c" gives accurate results for modal radius value up to 30.0 μm beyond which the computer gives errors due to the large amount of memory requirement in calculation of $D_n(\infty)$ by downward recurrence for large sized particles. Thus this chapter is devoted to developing a computer program for calculating volume scattering co-efficient $\beta(\theta)$ that could directly be used in the measurements obtained with the air quality monitoring system described in the next chapter.