3. Scattering of Radiation by Molecules and Particles

a. Introduction

Here, we'll deal with wave aspects of light rather than quantum aspects.

Consider components of electric field in 2 mutually perpendicular directions, parallel and perpendicular to the plane of propagation and propagating in the z direction:

$$\begin{split} E_r &= a_r e^{i(\omega t - kz)} & \omega = \text{circular frequency} \\ E_\ell &= a_\ell e^{i(\omega t - kz)} & k = \frac{2\pi}{\lambda} \end{split} \tag{1}$$

The intensity is given by:

$$I = E_r E_r^* + E_\ell E_\ell^* = a_r^2 + a_\ell^2$$
 (2)

Let us first consider <u>Single Scattering</u>. We may consider a single particle or a small volume of particles such that scattering events will all be single scattering events.

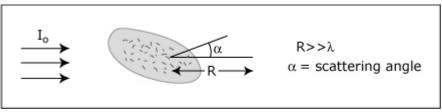


Fig. 1

 \vec{p} = phase matrix

$$p''$$
 = phase function

$$I = k_{sca} \vec{P} \vec{I}_0 \frac{dV}{4\pi R^2}$$
 or $I = h_{sca} \frac{P^{11} I_0 dV}{4\pi R^2}$

 k_{sca} = scattering cross-section per unit volume

$$\begin{split} k_{sca} &= \frac{\sigma_{sca}}{dV} = \frac{1}{dV} \sum_{i=1}^{N} \sigma_{sca}, \ i \\ & [k_{sca}] = length^{-1} \\ & [\sigma_{sca}] = length^{2} \\ & N = total \ no. \ of \ particles \\ Q_{sca,i} &= \frac{\sigma_{sca}, \ i}{G_{i}} \end{split}$$
 where G_{i} = geometrical cross section

$$Q_{sca} = \frac{\sigma_{sca}}{G} = \frac{\sum \sigma_{sca}, \ i}{\sum G_{i}}$$

$$Q_{sca} = Scattering \ efficiency$$

 \vec{P} is the phase matrix and provides the angular distribution and polarization of the scattered light. For our purpose here, lets consider the total intensity of the radiation whether polarized or not. Then the term, p^{11} , is the phase function or scattering diagram which defines the probability for scattering of unpolarized incident light in any direction. p^{11} is normalized such that:

$$\int \frac{p^{11} d\Omega}{4\pi} = 1 \quad \text{where } d\Omega = \text{element of solid angle}$$
 (3)

Let us define $<\cos\alpha> = \int\cos\alpha \; \frac{p^{11} \; d\Omega}{4\pi}$ where α is the scattering angle (see Fig. 1).

 $<\cos\alpha>=$ anisotropy parameter (or asymmetric parameter) and can vary between +1 and -1. $<\cos\alpha>=0$ for isotropic scattering.

We define analogous terms for particle absorption and we have:

$$\begin{aligned} k_{ext} &= k_{sca} + k_{abs} \\ \sigma_{ext} &= \sigma_{sca} + \sigma_{abs} \\ O_{ext} &= O_{sca} + O_{abs} \end{aligned} \qquad \sigma = \pi r^2 Q$$
 (4)

Then, we define:

$$\tilde{\omega} = \text{single scattering albedo} = \frac{k_{\text{sca}}}{k_{\text{ext}}} = \frac{\sigma_{\text{sca}}}{\sigma_{\text{ext}}} = \frac{Q_{\text{sca}}}{Q_{\text{ext}}}$$

For practical applications, k_{sca} and $\tilde{\omega}$ can be taken as constants and P^{11} is a function only of the scattering angle, α .

This special case is valid for:

- (1) randomly oriented particles, each of which has a plane of symmetry
- (2) randomly oriented asymmetric particles, if half the particles are mirror images of the others.
- (3) Rayleigh scattering and Mie scattering.

Another important definition: $\chi = \frac{2\pi a}{\lambda}$ where a = particle radius.

 $m = n_r - in_i$ where $n_r = real$ part of the index of refraction and $n_i = imaginary$ part. n_i is responsible for absorption and n_r is responsible for scattering.

For water, $n_{_{\!f}}=1.33$ across the visible and near infrared. And $n_{_{\!f}}$ will depend on the kinds of materials dissolved in the water drops. It will therefore be much more of a function of wavelength.

Returning to the analytical expression for the electric field as a beam of radiation passing through a single particle:

$$E(z, t) = E_0 e^{i(\omega t - kz)}$$

The intensity of radiation varies as the square of the E-field. So, we have:

$$I = E_0^2 e^{2i(\omega t - kz)} \qquad \qquad k = \frac{2\pi}{\lambda} \text{ and } \qquad \lambda = \frac{\lambda_0}{m}$$

So, we have: $E(z,t) = E_0 e^{i\left[\frac{-2\pi z}{\lambda_0}(n_r - in_l) + \omega t\right]}$

$$=E_{_0}\,e^{\frac{-2\pi z n_i}{\lambda_0}}\,\,e^{\,i\left(\frac{-2\pi z n_r}{\lambda_0}+\omega t\right)}$$

and
$$I=E_0^{\,2}\,\,e^{\,\left(\!\frac{-4\pi z n_i}{\lambda_0}\!\right)}\,\,e^{\,i\left(\!-\frac{4\pi z n_r}{\lambda_0}+2\omega t\right)}$$

and – using the definition of size parameter $\chi=\frac{2\pi a}{\lambda}$ where we will take z=2a= diameter of drop, we have:

$$I = E_0^2 e^{-4\chi n_i} e^{i(-4\chi n_i + z\omega t)}$$
absorption (5)

b. Mie scattering – still single scattering.

$$\begin{cases}
E_r^s \\
E_\ell^s
\end{cases} = \frac{\exp(-ikR + ikz)}{ikR} \begin{cases}
S_1(\alpha, \theta) S_4(\alpha, \theta) \\
S_3(\alpha, \theta) S_2(\alpha, \theta)
\end{cases} \begin{cases}
E_r^i \\
E_\ell^i
\end{cases}$$
(6)

If we consider isotropic, homogenous, spheres, we have:

$$\vec{S} = \begin{cases} S_1(\alpha) & 0 \\ 0 & S_2(\alpha) \end{cases} \qquad \vec{I} = \frac{1}{k^2 R^2} \vec{F} \vec{I}_0$$

And we have the transformation matrix:

The S values are in general complex number and functions of scattering angle.

$$\vec{F} = \begin{cases} \frac{1}{2} \left(S_1 S_1^* + S_2 S_2^* \right) & \frac{1}{2} \left(S_1 S_1^* - S_2 S_2^* \right) & 0 & 0 \\ \\ \frac{1}{2} \left(S_1 S_1^* - S_2 S_2^* \right) & \frac{1}{2} \left(S_1 S_1^* + S_2 S_2^* \right) & 0 & 0 \\ \\ 0 & 0 & \frac{1}{2} \left(S_1 S_2^* + S_2 S_1^* \right) & \frac{i}{2} \left(S_1 S_2^* - S_2 S_1^* \right) \\ \\ 0 & 0 & -\frac{i}{2} \left(S_1 S_2^* - S_2 S_1^* \right) & \frac{1}{2} \left(S_1 S_2^* + S_2 S_1^* \right) \end{cases}$$

which is proportional to the phase matrix: $\vec{F} = C \vec{P}$

(8)

The normalization condition on \vec{P} leads to: $C = \int_{4\pi}^{\pi} \frac{F^{11} d\Omega}{4\pi}$

and since σ_{sca} = effective cross section, we have:

$$\sigma_{sca} = \int_{4\pi} \frac{I R^2 d\Omega}{I_0} \qquad \qquad \text{and} \qquad \qquad C = \int_{4\pi} \frac{F^{11} \, d\Omega}{4\pi} = \frac{k^2 \sigma_{sca}}{4\pi} \, ,$$

where we've used $I=F^{11}/k^2R^2$

So - we have:

$$F^{11} = \frac{k^2 \sigma_{sca} p^{11}}{4\pi} = \frac{1}{2} (S_1 S_1^* + S_2 S_2^*) \blacktriangleleft \text{ defines phase function}$$

$$F^{21} = \frac{k^2 \sigma_{sca} p^{21}}{4\pi} = \frac{1}{2} (S_1 S_1^* - S_2 S_2^*) \tag{9}$$

$$F^{33} = \frac{k^2 \sigma_{sca} p^{21}}{4\pi} = \frac{1}{2} (S_1 S_2^* + S_2 S_1^*) \qquad F^{43} = \frac{k^2 \sigma_{sca} p^{43}}{4\pi} = -\frac{i}{2} (S_1 S_2^* - S_2 S_1^*)$$

For a single sphere, we have:

$$S_{1} = \sum_{n=1}^{\infty} \frac{2n+1}{n(n+1)} \left[a_{n} \pi_{n} + b_{n} \tau_{n} \right]$$

$$S_{2} = \sum_{n=1}^{\infty} \frac{2n+1}{n(n+1)} \left[b_{n} \pi_{n} + a_{n} \tau_{n} \right]$$
(10)

 π_n and τ_n are function only of α and relate to Legendre Polynomials.

 a_n and b_n are functions of $x=\frac{2\pi a}{\lambda}$ and $m=n_r-in_i$ and involve Spherical Bessel functions.

We also have:

$$Q_{sca} = \frac{2}{x^{2}} \sum_{n=1}^{\infty} (2n+1) (a_{n} a_{n}^{*} + b_{n} b_{n}^{*})$$

$$Q_{ext} = \frac{2}{x^{2}} \sum_{n=1}^{\infty} (2n+1) R_{e} (a_{n} + b_{n})$$

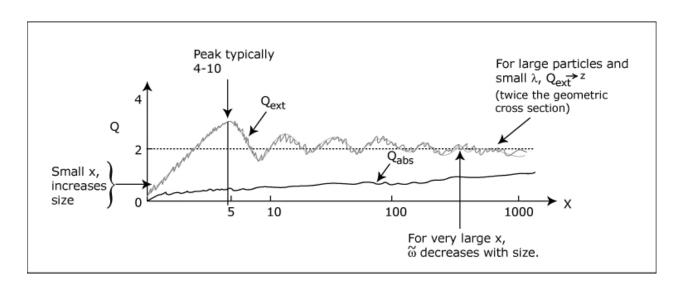
$$< \cos \alpha > = \frac{4}{x^{2} Q_{sca}} \sum_{n=1}^{\infty} \frac{n(n+2)}{n+1} R_{e} (a_{n} a_{n+1}^{*} + b_{n} b_{n+1}^{*}) + \frac{2n+1}{n(n+1)} R_{e} (a_{n} b_{n}^{*})$$
(11)

All above is for <u>Single Scattering</u> from a <u>Single Sphere</u>. In general, if optical thickness is not too large, single scattering can be applied to a distribution of particles assumed to be independent. We then have:

$$k_{sca} = \int_{r_{1}}^{r_{2}} \sigma_{sca}(r) n(r) dr = \int_{r_{1}}^{r_{2}} \pi r^{2} Q_{sca}(r) n(r) dr$$

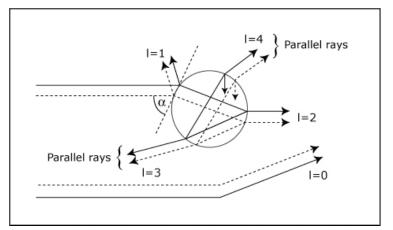
$$k_{ext} = \int_{r_{1}}^{r_{2}} \sigma_{ext}(r) n(r) dr = \int_{r_{1}}^{r_{2}} \pi r^{2} Q_{ext}(r) n(r) dr$$
(12)

where n(r) = size distribution, describing the number of the particles having radii between r and r+dr over the range r_1 to r_2 .



c. Geometric Optics:

When $r >> \lambda$, we can use ray theory of light due to Fresnel (see Van de Hulst, Ch. 3, <u>Light Scattering by Small Particles</u>). Terminology is:



0 - diffraction

1 - external reflection

2 - double refraction

3 - first rainbow

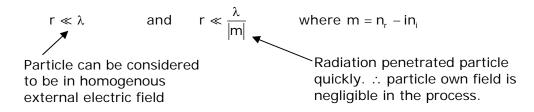
4 – second rainbow

and if $P(\theta) = \sum_{\ell=0}^{\infty} P_{\ell}(\theta)$, then $\frac{1}{4\pi} \int\limits_{0}^{2\pi} \int\limits_{0}^{\pi} P_{\ell}(\theta) \sin\theta \,d\theta \,d\phi$, is for non-absorbing spheres from Fresnel theory.

ℓ	real = 1.33	= <u>2.00</u>
0	.500	.500 \ always true in geometric optics
1	.033	.081 often sufficient to consider just
2	.442	.364 these
3	.020	.043
4	.033	.008
5	.002	.004

For non-absorbing particles, diffraction = $1\2$ of scattered light. Thus, the geometric optics limiting value of $Q_{ext} = 2.0$.

d. Rayleigh Scattering:



$$E_{sca} = \frac{k^2 \alpha_p E_{incident}}{R} sin \beta e^{-ikn}$$
 where β = angle between dipole moment and direction of scatter (13)

$$\vec{p}(\alpha) = \begin{cases} \frac{3}{\psi} (1 + \cos^2 \alpha) & -\frac{3}{\psi} \sin^2 \alpha & 0 & 0 \\ -\frac{3}{\psi} \sin^2 \alpha & \frac{3}{\psi} (1 + \cos^2 \alpha) & 0 & 0 \\ 0 & 0 & \frac{3}{2} \cos \alpha & 0 \\ 0 & 0 & 0 & \frac{3}{2} \cos \alpha \end{cases}$$
(14)

$$p^{11} = \frac{3}{\Psi} (1 + \cos^2 \alpha) \tag{15}$$

which gives angular distribution of intensity scattered by small particles – the Rayleigh scattering.

We also obtain:

$$Q_{sca} = \frac{8}{3} x^{4} \left| \frac{m^{2} - 1}{m^{2} + 2} \right| \qquad Q_{abs} = -4x I_{m} \left\{ \frac{m^{2} - 1}{m^{2} + 2} \right\}$$
 (16)

note that $Q_{abs} > Q_{sca}$ as $x \to 0$

note 4th power of x or λ^{-4} dependence This result is the same as Mie scattering as limiting case as $x \to 0$ (r<< λ).

12.815 Lecture Notes (Atmospheric Radiation)

Multiple Scattering

Refer back to Eq. 22 from the first set of Atmospheric Radiation lecture notes where we discussed Case III which arises due to the following two conditions:

$$F_{v0} >> B_{v}(T) \tag{1}$$

$$I(\theta',\phi',\tau_v) >> B_v(\tau_v) \tag{2}$$

The resulting equation of transfer is:

$$\mu \frac{dI_{v}}{d\tau_{v}}(\theta, \phi, \tau_{v}) = I_{v}(\theta, \phi, \tau_{v}) - J_{v}(\theta, \phi, \tau_{v})$$
(3)

$$\text{where} \quad J_{_{\boldsymbol{\nu}}}(\boldsymbol{\theta},\boldsymbol{\phi},\boldsymbol{\tau}_{_{\boldsymbol{\nu}}}) = \frac{\widetilde{\boldsymbol{\omega}}}{4\pi} \int P(\boldsymbol{\theta},\boldsymbol{\phi},\boldsymbol{\theta}',\boldsymbol{\phi}') \ I_{_{\boldsymbol{\nu}}}(\boldsymbol{\theta}',\boldsymbol{\phi}',\boldsymbol{\tau}_{_{\boldsymbol{\nu}}}) \sin \boldsymbol{\theta}' d\boldsymbol{\theta}' d\boldsymbol{\phi}' + \ \frac{\widetilde{\boldsymbol{\omega}}}{4} \, e^{-\tau_{_{\boldsymbol{\nu}}}/\mu_{_{\boldsymbol{\omega}}}} \ P(\boldsymbol{\theta}_{_{\boldsymbol{\omega}}},\boldsymbol{\phi}_{_{\boldsymbol{\omega}}}) \, F_{_{\boldsymbol{\nu}\odot}}$$

and the formal solution is:

$$\begin{split} I\left(\tau_{_{v}},\mu,\mu_{_{0}},\phi_{_{0}},\varphi\right) \uparrow &= \int\limits_{_{0}}^{\tau} J\left(\tau_{_{v}}\,',\mu,\mu_{_{0}},\varphi,\varphi_{_{0}}\right) e^{(\tau_{_{v}}-\tau_{_{v}}\,')/\mu} \, \frac{d\tau_{_{v}}\,'}{\mu} \quad \mu > 0 \\ I\left(\tau_{_{v}},\mu,\mu_{_{0}},\varphi,\varphi_{_{0}}\right) \downarrow &= -\int\limits_{_{T_{_{v}}}}^{\tau_{_{v_{s}}}} J\left(\tau_{_{v}}\,',\mu,\mu_{_{0}},\varphi,\varphi_{_{0}}\right) e^{-(\tau_{_{v}}\,'-\tau_{_{v}})/\mu} \, \frac{d\tau_{_{v}}\,'}{\mu} \quad \mu < 0 \end{split}$$

Due to the complexities of evaluating the integrals in Eq. 4, a number of techniques have been used to generate numerical results:

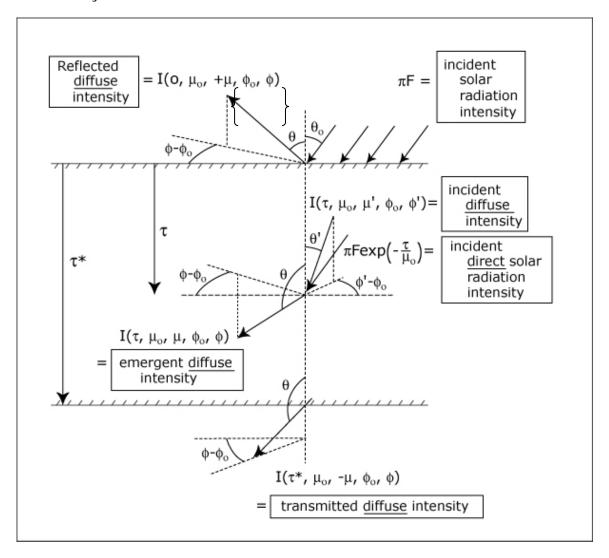
- 1. Discrete Ordinates
- 2. Doubling or Adding Method
- 3. Successive Orders of Scattering
- 4. Iteration of Formal Solution
- 5. Invariant Embedding
- 6. Method of X and Y Functions
- 7. Spherical Harmonics Method
- 8. Expansion in Eigenfunctions
- 9. Monte Carlo Method

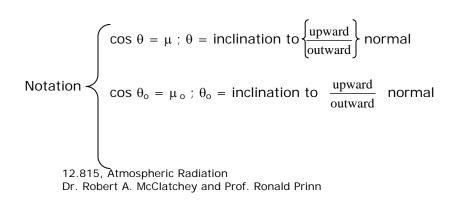
We will focus some attention on the Discrete Ordinates Method and apply an available computer program to some exercises.

Radiative Transfer in a Scattering Atmosphere

1. Coordinate system in a "plane parallel" atmosphere

Here <u>position</u> defined by z (or τ) <u>only</u>. Recall that optical depth τ related to altitude z by $d\tau = -\alpha dz$ where α is the extinction coefficient.





$$cos \; \theta' = \mu' \; ; \; \theta' = inclination \; to \left\{ \frac{upward}{outward} \right\} \; normal \;$$

From spherical geometry, the cosine of the scattering angle, α can be expressed in terms of the incoming and outgoing directions in the form:

$$\cos \alpha = \mu \mu' + (1 - \mu^2)^{1/2} (1 - \mu'^2)^{1/2} \cos(\phi' - \phi)$$
 (5)

Let us now digress for a moment and examine the properties of Legendre polynomials (which come to play in a variety of ways in radiative transfer problems).

We may consider writing the phase function in terms of Legendre polynomials in the form:

$$P(\cos \alpha) = \sum_{\ell=0}^{N} C_{\ell} P_{\ell} (\cos \alpha)$$
 (6)

Legendre polynomials have the following form, and orthogonal and recurrence properties:

$$\begin{split} P_{0}(\mu) &= 1 \qquad P_{n}(\mu) = \frac{1}{2^{n}n!} \, \frac{d^{n}}{d\mu^{n}} (\mu^{2} - 1)^{n} \qquad (n = 1, 2, \dots) \\ So, \qquad P_{1}(\mu) &= \mu \qquad P_{2}(\mu) = \frac{3}{2} \mu^{2} - \frac{1}{2} \qquad \dots \\ \int_{-1}^{1} P_{\ell}(\mu) \, P_{k}(\mu) \, d\mu &= \begin{cases} 0 & \ell \neq h \\ \frac{2}{2\ell + 1} & \ell = h \end{cases} \end{split} \tag{7}$$

$$\mu P_{\ell}(h) &= \frac{\ell + 1}{2\ell + 1} \, P(\mu) + \frac{\ell}{2\ell + 1} \, P(\mu)$$

Using Eq. 5, the Phase Function defined above may be written as follows:

$$P(\mu, \theta, \mu', \phi') = \sum_{\ell=0}^{N} C_{\ell} P_{\ell} \left[\mu \mu' + (1 - \mu^{2})^{\frac{1}{2}} (1 - \mu')^{\frac{1}{2}} \cos(\theta' - \theta) \right]$$
 (8)

From the orthogonality condition, the expansion coefficients are given by:

$$C_{\ell} = \frac{2\ell+1}{2} \int_{-1}^{1} P\left(\mu\right) P_{\ell}\left(\mu\right) d\mu \qquad \qquad \ell = 0, 1 \dots ... N$$

where we note that the phase function is normalized to unity:

$$\frac{1}{4\pi}\int_{0}^{2\pi}\int_{-1}^{1}P\left(\mu\right)d\mu\,d\phi\equiv1$$

There is an addition theorem for Legendre polynomials which allows us to write the Phase Function as follows:

$$P(\mu, \phi, \mu', \phi') = \sum_{m=0}^{N} \sum_{\ell=0}^{N} C_{\ell}^{m} P_{\ell}^{m} (\mu) P_{\ell}^{m} (\mu') \cos m (\phi' - \phi)$$

$$(9)$$

where P_{ℓ}^{m} denotes the Associated Legendre polynomials and:

$$C_{\ell}^{m}(2-\delta_{0,m})C_{\ell}\frac{\left(\ell-m\right)!}{\left(\ell+m\right)!}, \quad \ell=m,\ldots..N \qquad 0 \leq m \leq n \tag{10}$$

$$\delta_{0,m}=\begin{cases} 1, & m=0\\ 0, & \text{otherwise} \end{cases}$$

In view of the expansion of the phase function, the diffuse intensity may also be expanded in a cosine series in the form:

$$I(\tau, \mu, \phi) = \sum_{m=0}^{N} I^{m}(\tau, \mu) \cos m(\phi_{0} - \phi)$$
(11)

Substituting Eqs. 9 and 11 into Eq. 3, and using the orthogonality of the associated Legendre polynomials, the equation of transfer splits into (N+1) independent equations, and may be written as:

$$\mu \frac{dI^{m}(\tau, \mu)}{d\tau} = I^{m}(\tau, \mu) - (1 + \delta_{0,m}) \frac{\tilde{\omega}}{4} \sum_{\ell=m}^{N} C_{\ell}^{m} P_{\ell}^{m}(\mu)$$

$$\times \int_{-1}^{1} P_{\ell}^{m}(\mu') I^{m}(\tau, \mu') d\mu'$$

$$- \frac{\tilde{\omega}}{4\pi} \sum_{\ell=0}^{N} C_{\ell}^{m} P_{\ell}^{m}(\mu) P_{\ell}^{m}(-\mu_{0}) F_{o} e^{-\frac{\tau}{\mu_{0}}}$$
(12)

m = 0, 1, N

Let us rewrite these equations as follows:

$$\mu \frac{dI^{m}(\tau, \mu)}{d\tau} = I^{m}(\tau, \mu) - J^{m}(\tau, \mu)$$
(13)

with the source function given by:

$$J^{m}(\tau, \mu) = (1 + \delta_{0,m}) \frac{\tilde{\omega}}{4} \sum_{\ell=m}^{N} C_{\ell}^{m} P_{\ell}^{m} (\mu) \int_{-1}^{1} P_{\ell}^{m}(\mu') I^{m}(\tau, \mu') d\mu' + \frac{\tilde{\omega}}{4\pi} \sum_{\ell=m}^{N} C_{\ell}^{m} P_{\ell}^{m} (\mu) P_{\ell}^{m} (-\mu_{0}) F_{0} e^{-\frac{\tau}{\mu_{0}}}$$
(14)

To proceed with the solution of Eq. 13, we first <u>discretize</u> the equation by replacing μ with μ_i (i= -n,...., n, with n= 1, 2,....) and the integral with a sum with the weights, a_i

$$\int_{-1}^{1} f(\mu) d\mu = \sum_{j=-n}^{n} f(\mu_{j}) a_{j}$$
 (15)

The homogeneous solution for the set of first-order differential equations may be written:

$$I^{m}(\tau, \mu_{i}) = \sum_{i=-n}^{n} L_{j}^{m} \psi_{j}^{m} (\mu_{i}) e^{-k_{j}^{m} \tau}$$
(16)

where $\psi_j^m(\mu_i)$ and k_j^m denote the eigenvectors and eigenvalues, respectively, and L_j^m are coefficients to be determined from appropriate boundary conditions. On substituting Eq. 16 into the homogeneous part of Eq. 13, the eigenvectors may be expressed by

$$\psi_{j}^{m}(\mu_{i}) = \frac{(1 + \delta_{0,m})\tilde{\omega}}{4(1 + \mu_{i} K_{i}^{m})} \sum_{\ell=m}^{N} C_{\ell}^{m} P_{\ell}^{m}(\mu_{i}) \sum_{q=-n}^{n} a_{q} P_{\ell}^{m}(\mu_{q}) \psi_{j}^{m}(\mu_{q})$$
(17)

The particular solution may be written in the form

$$I_{n}^{m}(\tau, \mu_{i}) = Z^{m}(\mu_{i}) e^{-\tau/\mu_{0}}$$
(18)

From Eq. 13, we have

$$Z^{m}(\mu_{i}) = \frac{\tilde{\omega}}{4\left(1 + \frac{\mu_{j}}{\mu_{0}}\right)} \sum_{\ell=m}^{N} C_{\ell}^{m} P_{\ell}^{m}(\mu_{i})$$
(19)

$$X \left(\sum_{q=-n}^{n} a_{q} P_{\ell}^{m}(\mu_{q}) Z^{m}(\mu_{q}) + P_{\ell}^{m}(-\mu_{0}) \frac{F_{\odot}}{\pi} \right)$$

Equations 17 and 19 are linear equations in Ψ_j^m and z^m and may be solved numerically. The complete solution for Eq. 13 is the sum of the general

solution for the associated homogeneous system of the differential equations and the particular solution. Thus,

$$I^{m}(\tau, \mu_{i}) = \sum_{j=-n}^{n} L_{j}^{m} \psi_{j}^{m} (\mu_{i}) e^{-k_{j}^{m} \tau} + Z^{m}(\mu_{i}) e^{-\tau / \mu_{0}}$$

$$i = -n, \dots + n$$
(20)

In order to determine the unknown coefficients, L_j^m , a_q , boundary conditions must be imposed.

In the discrete-ordinates method for radiative transfer, analytical solutions for the diffuse intensity are explicitly given for any optical depth. Thus the internal radiation field can be evaluated without additional computational effort. And furthermore, useful approximations can be developed from this method for flux calculations.

Advantages of Discrete Ordinate Method

- a) In principle numerical computations can be done for any order of approximation.
- b) The internal radiation field is determined not just the Reflection & Transmission.
- c) Accurate results (to about 1%) are achievable with only a few streams (3-4) for most cases.

We will utilize the Discrete Ordinate computer program to do a few excercises.

Multiple Scattering Computational Techniques

1. Discrete Ordinates (We'll discuss in detail in a few minutes.)

2. Doubling or Adding

Principle: If reflection and transmission is known for each of two layers, the reflection and transmission from the combined layer can be obtained by computing the successive reflections back and forth between the two layers. If the two layers are chosen to be identical, the results for a thick homogenous layer can be built up rapidly in a geometric (doubling) manner.

3. Successive Orders of Scattering

Principle: Intensity is computed individually for photons scattered once, twice, three times, etc. with the total intensity obtained as the sum over all orders. If the intensity is expanded in a Fourier series, the high frequency terms arise from photons scattered a small number of times. Therefore, most Fourier terms can be obtained with some accuracy by computing a few orders of scattering.

4. Iteration of Formal Solution

Direct solution of integral over source function by dividing atmosphere into layers with small optical thickness.

5. Invariant Imbedding

Differential Equations are developed which give the change of reflection and transmission matrices when an optically thin layer is added to the atmosphere. It is a special case of the Doubling or Adding technique.

6. Method of X and Y Functions

Involves the determination of integral equations for functions which depend upon only one angle and are directly related to Reflection and Transmission matrices. The integral equations need to be solved numerically. The integral equations are completely specified by a <u>character function</u> depending on the particular phase function. This method is due to Chandrasekhar.

7. Spherical Harmonic Method

Intensity is immediately expanded into a finite number of spherical harmonics and then the Phase Function is expanded in Legendre polynomials similar to the Discrete Ordinate method.

8. Expansion in Eigenfunctions

Standard technique for solving differential equations. Find homogenous solution and particular solution. Apply boundary condition. Direct application to complete RTE is ponderous. Discrete Ordinates technique depends on this approach for solving discretized set of equations.

9. Monte Carlo Method

Scattering of an individual photon can be considered to be a stochastic process, with the Phase Function being the probability density function for scattering at a given angle. Photons are allowed to play a game of chance in a computer and by recording the history of a sufficient number of photons, the radiation field can in principle be determined to an arbitrary accuracy. The basic simplicity of this method allows great flexibility, and hence it can be applied to complicated problems which would be virtually insoluble by other methods.

Isotropic Scattering and Discrete Ordinates

Pertinent RTE:

$$\begin{split} \mu\,dI\left(\mu,\,\phi,\,\tau\right)\,/\,d\tau &=\,I\left(\mu,\,\phi,\,\tau\right) - \frac{\tilde{\omega}}{4\pi} \iint P\left(\mu,\,\phi,\,\mu',\,\phi'\right)\,\,I\left(\mu',\,\phi',\,\tau\right) d\mu'\,d\phi' \\ &+ \frac{\tilde{\omega}}{4}\,e^{-\frac{\tau}{\mu_0}}\,P\left(\mu_0\,,\,\phi_0\right)F_\odot \end{split} \tag{1}$$

For isotropic scattering, we have:

$$P(\mu, \phi, \mu', \phi') = 1 \text{ and } I(\mu, \tau) = \frac{1}{2\pi} \int_{0}^{2\pi} I(\mu, \phi, \tau) d\phi$$
 (2)

i.e. - Intensity is azimuthally independent.

$$\mu \frac{dI\left(\tau,\mu\right)}{d\tau} = I\left(\tau,\mu\right) - \frac{\tilde{\omega}}{2} \int_{-1}^{1} I\left(\tau,\mu'\right) d\mu' - \frac{\tilde{\omega}}{4\pi} F_{\odot} e^{-\frac{\tau}{\mu_{0}}} \tag{3}$$

Applying Gaussian Quadrature, and setting $I_i = I(\tau, \mu_i)$, we have:

$$\mu_{i} \frac{dI_{i}}{d\tau} = I_{i} - \frac{\tilde{\omega}}{2} \sum_{j=-n}^{+n} I_{j} a_{j} - \frac{\tilde{\omega}}{4\pi} F_{\odot} e^{-\frac{\tau}{\mu_{0}}}$$

$$i = -n, \dots, +n$$

$$(4)$$

Since this is <u>linear differential equation</u>, we need to seek the <u>general solution</u> (sometimes called the homogenous solution) and then the <u>particular solution</u>.

Homogenous solution:

Try (guess) $I_i = g_i e^{-k\tau}$ where g_i and k are constants.

$$\mu_{i} \frac{dI_{i}}{d\tau} = I_{i} - \frac{\tilde{\omega}}{2} \sum_{i} I_{j} a_{j}$$
 (5)

$$\therefore \ g_i \ (1 + \mu_i \ k) = \frac{\tilde{\omega}}{2} \ \sum_j a_j \ g_i$$

So, g_i must be of the form $L/(1 + \mu_i k)$ where L is a constant.

Substituting this back into Eq. 5, we get the characteristic equation for eigenvalue k

$$\frac{\tilde{\omega}}{2} \sum_{j=-n}^{+n} \frac{a_j}{(1+\mu_j k)} = \tilde{\omega} \sum_{j=1}^{n} \frac{a_j}{(1-\mu_j^2 k^2)} = 1$$
Note difference in summation (6)

This Eq. has 2n roots, $\pm k_{\alpha}$ α = 1......n which when $\tilde{\omega}$ = 1 includes $2K_{\alpha}$ values of zero.

General Solution is:

$$I_{i} = \sum_{\alpha=1}^{n} \frac{L \pm \alpha \ e^{\mp k_{\alpha}\tau}}{1 \pm \mu_{i}k_{\alpha}} \qquad \qquad i = -n, \dots, +n$$
 (7)

Particular Solution:

Try:
$$I_i = \frac{\tilde{\omega}}{4\pi} F_{\odot} h_i e^{-\tau/\mu_0}$$
 $i = -n, \dots, +n$

We have:
$$\frac{-\mu_i}{\mu_0} \, h_i = h_i - \frac{1}{2} \, \widetilde{\omega} \sum_{j=-n}^{+n} a_j h_j \, -1$$

or
$$h_i \left(1 + \frac{\mu_i}{\mu_0} \right) = \frac{\tilde{\omega}}{2} \sum_{j=-n}^{+n} a_j h_j + 1$$
 (8)

$$h_i$$
 must be of the form = $\frac{\gamma}{1 + \frac{\mu_i}{\mu_0}}$ (9)

with
$$\gamma = \left(1 - \tilde{\omega} \sum_{j=1}^{n} \frac{a_{j}}{[1 - \mu_{i} 4\mu_{0}^{2}]}\right)^{-1}$$
 (10)

Adding the homogenous and particular solutions, we obtain:

$$I_{i} = \sum_{j=1}^{n} \frac{L_{j} e^{-k_{j}\tau}}{1 + \mu_{i} k_{j}} + \frac{\tilde{\omega} F_{\odot} \gamma e^{-\tilde{\gamma} \mu_{0}}}{4\pi \left(1 + \frac{\mu_{i}}{\mu_{0}}\right)}$$

$$i = -n, \dots + n$$
(11)

The L_i are determined from boundary conditions.