A NUMERICAL METHOD FOR CALCULATING THE MEAN INTENSITY IN AN INHOMOGENEOUS RAYLEIGH SCATTERING ATMOSPHERE

YUK L. YUNG

Center for Earth and Planetary Physics, Harvard University, Cambridge, MA 02138, U.S.A.

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Abstract—We describe a method for calculating directly the mean integrated intensity in an inhomogeneous Rayleigh scattering atmosphere using a combined variational and iterative technique. This method is particularly useful for computing dissociation rates in aeronomical problems. Simple semi-analytic expressions are derived.

1. INTRODUCTION

The importance of Rayleigh scattering on photochemical processes in the stratosphere has been pointed out by Callis. The correction to the direct solar beam due to multiple scattering in calculating dissociation rates for species like NO₂ and H₂O₂ may be significant (Wofsy, private communication). The important quantity of interest is the integrated intensity

\[ J = \int_{-1}^{1} \int_{0}^{2\pi} I(\mu, \phi) \, d\mu \, d\phi. \]

Most methods for calculating Rayleigh scattering are quite involved and do not determine \( J \) directly. It is the purpose of this paper to point out a conceptually simple and computationally efficient method that yields \( J \) directly in terms of elementary functions and a few parameters.

2. THEORY

The equation of radiative transfer for a Rayleigh scattering atmosphere including polarization has been formulated by Chandrasekhar. We shall follow his notation. For our present problem, we are only interested in the mean intensity and only need to deal with two \( \phi \)-independent components of the Stokes vector \((I_I, I_\nu)\). Assuming a plane parallel geometry (see Fig. 1(a)), the equation of radiative transfer is

\[
\frac{d}{d\tau} \left[ I (\tau, \mu) \right] = \left[ I (\tau, \mu) \right] - \frac{3}{8} \tilde{\omega}(\tau) \int_{-1}^{1} \left[ \frac{2(1-\mu^2)(1-\mu'^2) + \mu^2 \mu'^2}{\mu'^2} \right] \left[ I (\tau, \mu') \right] \, d\mu',
\]

where \( \tau \) is the optical depth, \( \tilde{\omega}(\tau) \) the single scattering albedo, and \( \mu \) the cosine of the zenith angle.

If we assume that the incident sunlight is unpolarized, and that the surface reflects according to Lambert's law with albedo \( \lambda \), then we have the following boundary conditions at \( \tau = 0 \) and \( \tau = \tau^* \):

\[
I^- (0, \mu) = I^- (0, \mu) = \frac{E}{4 \delta} \delta (\mu - \mu_0),
\]

\[
I^+ (\tau^*, \mu) = I^+ (\tau^*, \mu) = \lambda \int_{0}^{1} \mu' (I^- (\tau^*, \mu') + I^- (\tau^*, \mu')) \, d\mu'.
\]

We shall transform eqn (1) into an integral equation. We define

\[
J_\tau (\tau) = \frac{3}{8} \tilde{\omega}(\tau) \int_{-1}^{1} (1 - \mu'^2) I (\tau, \mu') \, d\mu',
\]

\[
J_\sigma (\tau) = -\frac{3}{8} \tilde{\omega}(\tau) \int_{-1}^{1} \mu'^2 I (\tau, \mu') + I (\tau, \mu') \, d\mu'.
\]
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Fig. 1(a). Geometry of the radiative transfer problem: $\pi F = \text{incident solar flux}$, $\mu_0 = \text{cosine of solar zenith angle}$, $\tau^* = \text{optical thickness}$, $\bar{\omega}(\tau) = \text{single scattering albedo}$, and $\lambda = \text{Lambert surface albedo}$; (b) Schematic diagram of a scattering medium divided into $N$ layers.

Following a procedure similar to that described in YUNG and GOODY,\(^{(1)}\) we can derive the following integral equation for $I_2(\tau)$:

$$I_2(\tau) = \int_0^\tau \left[ \frac{3E_\tau}{32} e^{-\mu_0 F} \left( 1 - \mu_0^2 \right) + \frac{3\mu_0 \bar{\omega}(\tau)}{16} e^{-\mu_0 F} \left( E_2 - E_4 \right) \right] ds$$

In the above equation, $[E_n]_{\tau-s} = E_n(\tau - s)$, $[E_n]_{\tau-s} = E_n(\tau^* - s)$, and $[E_n]_{\tau-s} = E_n(\tau^* - s)$. The function $E_n(x)$ is the exponential integral defined by CHANDRASEKHAR\(^{(2)}\) (see the Appendix). It should be noted that the integral eqn (4) is exactly equivalent to eqn (1) with boundary conditions (2). We have not introduced any approximation yet. The mean integrated intensity $J(\tau)$ is readily expressed in terms of $I_1(\tau)$ and $I_2(\tau)$, viz.

$$J(\tau) = 2\pi \int_0^\tau I_1(\tau, \mu') + I_2(\tau, \mu') d\mu'$$

To solve eqn (4) approximately, we shall use a method first applied by SZE\(^{(3)}\) to isotropic scattering. We divide the scattering medium into $N$ layers, each of thickness $\Delta$, and single scattering albedo $\bar{\omega}$, as illustrated in Fig. 1(b). We shall initially assume that the values of $J_1(\tau)$ and $J_2(\tau)$ in the $i$th layer are, respectively, some constants $\Gamma_1^i$ and $\Gamma_2^i$ which will be determined subsequently. Substituting for $J_1(\tau)$ and $J_2(\tau)$ in eqn (4) we replace eqn (4) by a system $2N \times 2N$ equations.
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The equality can never be satisfied for the entire interval. However, we can adjust the constants $\Gamma_i^1$ and $\Gamma_i^2$ such that the error

$$\epsilon_{1i}(\tau) = \Gamma_i^1 - R_i^1(\tau),$$
$$\epsilon_{2i}(\tau) = \Gamma_i^2 - R_i^2(\tau),$$

is a minimum over each $i$th layer. This gives us $2N$ conditions to determine the $2N$ constants $\{\Gamma_i^1, \Gamma_i^2\}_{i=1,N}$. It can be shown that the minimum condition is achieved by

$$\langle \epsilon_{1i}(\tau) \rangle_i = 0,$$
$$\langle \epsilon_{2i}(\tau) \rangle_i = 0,$$

where $\langle \rangle_i$ denote average over the $i$th layer. In this case, the $\Gamma_i^1$ and $\Gamma_i^2$ are determined by the following $2N \times 2N$ matrix:

$$\begin{bmatrix}
\delta_{ij} - A_{1i}(i,j) & -A_{2i}(i,j) \\
-A_{2i}(i,j) & \delta_{ij} - A_{2i}(i,j)
\end{bmatrix}
\begin{bmatrix}
\Gamma_i^1 \\
\Gamma_i^2
\end{bmatrix}
= \begin{bmatrix}
f_i^1 \\
f_i^2
\end{bmatrix}, \quad (6)$$

where

$$f_i^1 = \frac{3\omega_0F_i^1}{2\Delta_i} \{1 - \mu_i \epsilon(\mu_i) e^{-\mu_i \epsilon}\},$$
$$f_i^2 = \frac{3\omega_0F_i^2}{2\Delta_i} \{1 + \mu_i \epsilon(\mu_i) e^{-\mu_i \epsilon}\},$$

$$A_{1i}(i,j) = \frac{3\omega_i}{4\Delta_i} \{m_{i1}^1 - 2m_{i2}^1 + m_{i3}^1 + \lambda (l_i^2 - l_i^4)(l_i^2 - l_i^4)),
$$
$$A_{2i}(i,j) = \frac{3\omega_i}{8\Delta_i} \{m_{i1}^1 - m_{i2}^1 + \lambda (l_i^2 - l_i^4)(l_i^2 - l_i^4)),
$$
$$A_{2i}(i,j) = \frac{3\omega_i}{4\Delta_i} \{m_{i1}^1 - m_{i2}^1 + \lambda (l_i^2 - l_i^4)(l_i^2 - l_i^4)),
$$
$$A_{2i}(i,j) = \frac{3\omega_i}{8\Delta_i} \{m_{i1}^1 + m_{i2}^1 + \lambda (l_i^2 + l_i^4)(l_i^2 + l_i^4)).
$$

The integrals of $E_\mathbf{a}$ function over appropriate layers, $l_i^*$ and $m_{i2}^1$ are defined in the Appendix. We shall solve eqn (4) with $F = 1$. Having obtained $\Gamma_i^1$ and $\Gamma_i^2$, it is easy to show from eqn (5) that

$$\frac{J(\tau)}{\pi F} = e^{-\mu_i} + \Lambda(\tau),$$
$$\Lambda(\tau) = 2\lambda \mu_0 [e^{-\lambda(\mu_i)}] E_\mathbf{a}(\tau^* - \tau)$$
$$+ 2 \sum_{i=1}^N (2\Gamma_i^1 + \Gamma_i^2) \gamma_i^1(\tau) - (2\Gamma_i^1 - \Gamma_i^2) \gamma_i^2(\tau)$$
$$+ 4\lambda E_\mathbf{a}(\tau^* - \tau) \sum_{i=1}^N (2\Gamma_i^1 + \Gamma_i^2) \gamma_i^3(\tau) - (2\Gamma_i^1 - \Gamma_i^2) \gamma_i^4(\tau),$$

where we have defined $\Lambda(\tau)$ such that $\Lambda(0)$ is the same as "$\Lambda$" in McElroy and Hunt, while $\gamma_i^\mathbf{a}(\tau)$ is defined in the Appendix.

The meaning of eqns (7) and (8) is easy to understand. The first term on the right hand side is the attenuated direct solar beam. The correction term $\Lambda(\tau)$ consists of three parts. The first part is the diffused sun reflected from the ground. The second and third parts are each a sum, arising from Rayleigh scattering of the direct and reflected beams respectively.

In the limit $\mu_0 \tau^* \ll 1$, the one layer approximation is highly accurate and merits a special
discussion because of its simplicity. \( \Gamma_1 \) and \( \Gamma_2 \) are given by

\[
\begin{bmatrix}
1 - A_{11} & -A_{12} \\
-A_{21} & 1 - A_{22}
\end{bmatrix}
\begin{bmatrix}
\Gamma_1 \\
\Gamma_2
\end{bmatrix}
= \begin{bmatrix}
f_1 \\
f_2
\end{bmatrix},
\]

(9)

where

\[
f_1 = \frac{3 \hat{\omega} \mu_0}{32 \pi^2} F \left[ (1 - \mu_0^2) \left( 1 - e^{-\mu_0} \right) + 2 \lambda e^{-\mu_0} \left( \frac{1}{4} - E_s(\tau^*) + E_d(\tau^*) \right) \right],
\]

\[
f_2 = \frac{3 \hat{\omega} \mu_0}{32 \pi^2} F \left[ (1 + \mu_0^2) \left( 1 - e^{-\mu_0} \right) + 2 \lambda e^{-\mu_0} \left( \frac{3}{4} - E_d(\tau^*) - E_s(\tau^*) \right) \right],
\]

\[
A_{11} = \frac{3 \hat{\omega}}{4\pi^2} \left[ 2 \left( \frac{8}{15} \tau^* - \frac{1}{12} + E_s(\tau^*) - 2 E_d(\tau^*) + E_d(\tau^*) \right)
\]

\[
\quad + \lambda \left( \frac{1}{4} - E_d(\tau^*) + E_d(\tau^*) \right) \right],
\]

\[
A_{12} = \frac{3 \hat{\omega}}{4\pi^2} \left[ \left( \frac{2}{15} \tau^* - \frac{1}{12} + E_s(\tau^*) - E_s(\tau^*) \right)
\]

\[
\quad + \lambda \left( \frac{1}{4} - E_s(\tau^*) + E_s(\tau^*) \right) \right],
\]

\[
A_{21} = \frac{3 \hat{\omega}}{4\pi^2} \left[ 2 \left( \frac{2}{15} \tau^* - \frac{1}{12} + E_s(\tau^*) - E_s(\tau^*) \right)
\]

\[
\quad + \lambda \left( \frac{1}{4} - E_s(\tau^*) + E_s(\tau^*) \right) \right],
\]

\[
A_{22} = \frac{3 \hat{\omega}}{4\pi^2} \left[ \left( \frac{6}{5} \tau^* - \frac{2}{3} + E_s(\tau^*) + E_s(\tau^*) \right)
\]

\[
\quad + \lambda \left( \frac{3}{4} - E_s(\tau^*) - E_s(\tau^*) \right) \right].
\]

The solution to \( \Lambda(\tau) \) is given by

\[
\Lambda(\tau) = 2 \lambda \mu_0 e^{-\mu_0} E_s(\tau^* - \tau)
\]

\[
\quad + 4 \Gamma \left[ \frac{4}{3} - E_s(\tau) + E_d(\tau) - E_s(\tau^* - \tau) + E_d(\tau^* - \tau) \right]
\]

\[
\quad + 2 \lambda E_d(\tau^* - \tau) \left( \frac{1}{2} - E_d(\tau) + E_d(\tau) - E_s(\tau^* - \tau) + E_s(\tau^* - \tau) \right)
\]

\[
\quad + 2 \Gamma \left[ \frac{8}{3} - E_s(\tau) - E_d(\tau) - E_s(\tau^* - \tau) - E_d(\tau^* - \tau) \right]
\]

\[
\quad + 2 \lambda E_d(\tau^* - \tau) \left( \frac{3}{2} - E_s(\tau) - E_s(\tau) - E_d(\tau^* - \tau) - E_s(\tau^* - \tau) \right).\]

(10)

Given a table of \( E_s(x) \) functions, we can actually compute \( \Lambda(\tau) \) by hand!

3. RESULTS AND DISCUSSION

A computer program was developed to calculate \( \Lambda(\tau) \) for an arbitrary number of levels. For simplicity, we have chosen equal spacing for all of the levels. Figure 2 shows the result for \( \Lambda(\tau) \) with \( \tau^* = 0.5, \mu_0 = 0.5, \lambda = 0.25 \) and \( \omega = 0.5, 1 \). The solid curve is computed by choosing \( N = 30 \), and the dashed curve is computed with \( N = 1 \). Figure 3 shows a similar calculation with \( \tau^* = 0.5, \mu_0 = 0.1, \lambda = 0.25 \) and \( \omega = 0.5, 1 \). The solid curve and the dashed curve represent results with \( N = 30 \) and \( 3 \), respectively. It is clear that the merit of this method lies in the fact that we only require a relatively small number of levels to ensure a reasonable answer. The absolute accuracy is checked with results obtained by using the tables of COULSON et al.

(7) for homogeneous, conservative scattering. We can only check \( \Lambda(0) \) and \( \Lambda(\tau^*) \) because only the reflected and transmitted intensities have been tabulated. Tables 1 and 2 show the results of such a comparison for a fairly representative range of parameters. For \( \sim 10\% \) accuracy in \( \Lambda(\tau) \), one level is sufficient.
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Fig. 2. $\Lambda(\tau)$ calculated with $\tau^* = 0.5$, $\mu_0 = 0.5$, $\lambda = 0.25$ and $\sigma = 0.1$. The solid line has been computed with $N = 30$ and the dashed line with $N = 1$.

Fig. 3. $\Lambda(\tau)$ calculated with the same parameters as in Fig. 2 except that $\mu_0$ was chosen to be 0.1 and $N$ for the dashed line was 3.

Table 1. Comparison of approximate values for $\Lambda(0)$ and $\Lambda(\tau^*)$ calculated from a 1-layer approximation with those obtained from the tables of COULSON et al.\(^{(7)}\)

<table>
<thead>
<tr>
<th>$\tau^*$</th>
<th>$\mu_0$</th>
<th>$\lambda$ = 0</th>
<th>$\lambda$ = 0.25</th>
<th>$\lambda$ = 0.50</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Exact</td>
<td>Approx</td>
<td>Err(%)</td>
<td>Exact</td>
</tr>
<tr>
<td>0.10</td>
<td>0.02</td>
<td>0.0454</td>
<td>0.0450</td>
<td>0.0880</td>
</tr>
<tr>
<td>0.25</td>
<td></td>
<td>0.1698</td>
<td>0.1364</td>
<td>0.1891</td>
</tr>
<tr>
<td>0.40</td>
<td>0.02</td>
<td>0.0471</td>
<td>0.0467</td>
<td>0.2345</td>
</tr>
<tr>
<td>0.25</td>
<td>0.2837</td>
<td>0.2693</td>
<td>-5.4</td>
<td>0.4023</td>
</tr>
<tr>
<td>0.92</td>
<td>0.02</td>
<td>0.0395</td>
<td>0.0392</td>
<td>0.4765</td>
</tr>
<tr>
<td>0.25</td>
<td>0.2793</td>
<td>0.2732</td>
<td>-2.2</td>
<td>0.5972</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>$\Lambda(\tau^*)$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\tau^*$</td>
</tr>
<tr>
<td>----------</td>
</tr>
<tr>
<td></td>
</tr>
<tr>
<td>0.10</td>
</tr>
<tr>
<td>0.25</td>
</tr>
<tr>
<td>0.40</td>
</tr>
<tr>
<td>0.25</td>
</tr>
<tr>
<td>0.92</td>
</tr>
<tr>
<td>0.25</td>
</tr>
</tbody>
</table>
Table 2. Comparison of approximate values for $A(0)$ and $\Lambda r^*$ calculated from a 4-layer approximation with those obtained from the tables of COULSON et al.*

<table>
<thead>
<tr>
<th>$\tau/\mu_0$</th>
<th>$\tau/\mu_0 = 0$</th>
<th>$\tau/\mu_0 = 0.25$</th>
<th>$\tau/\mu_0 = 0.80$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Exact</td>
<td>Approx</td>
<td>Error (%)</td>
<td>Exact</td>
</tr>
<tr>
<td>0.10</td>
<td>0.02</td>
<td>0.0545</td>
<td>0.0455</td>
</tr>
<tr>
<td>0.25</td>
<td>0.1698</td>
<td>0.1415</td>
<td>-11.3</td>
</tr>
<tr>
<td>1.00</td>
<td>0.5146</td>
<td>0.5040</td>
<td>-2.2</td>
</tr>
<tr>
<td>4.40</td>
<td>0.92</td>
<td>0.4646</td>
<td>0.4646</td>
</tr>
<tr>
<td>1.00</td>
<td>0.5467</td>
<td>0.5120</td>
<td>-6.6</td>
</tr>
<tr>
<td>1.00</td>
<td>0.5467</td>
<td>0.5120</td>
<td>-6.6</td>
</tr>
<tr>
<td>0.92</td>
<td>0.3955</td>
<td>0.3955</td>
<td>0.5</td>
</tr>
<tr>
<td>0.25</td>
<td>0.3293</td>
<td>0.3293</td>
<td>-0.1</td>
</tr>
<tr>
<td>1.00</td>
<td>0.6907</td>
<td>0.6886</td>
<td>0.2</td>
</tr>
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</table>

for $\tau/\mu_0 < 1$ and, even for $\tau/\mu_0 \approx 10$, we note that four levels are sufficient. For non-conservative scattering, $\omega_l < 1$ and our accuracy is expected to improve.

We shall discuss some special mathematical properties of eqns (6) and (7) and how they can be exploited to economize on computing time. We may note that the matrix on the right-hand side of eqn (6) does not contain the parameter $\mu_0$. Thus, if we are interested in the diurnal change in $A(\tau)$, we can save the inverse of this matrix and calculate the new $T_i'$ and $T_i^z$ just by changing $\tau'$ and $\tau^z$.

The quantities $y_n(x)$, $l^*$, and $m_i^*$ are mainly determined by $T_*$ and $N$, the number of levels, and may be saved for future computations that only involve a change in $\lambda$ or $\omega$. Most of the time expended in this program is in evaluating the $E_n(x)$ functions and in inverting the matrix in eqn (6). We should note that, if the levels are equally spaced, the dominant terms in the matrix in eqn (6) all occur on the diagonal. The time for performing a typical calculation once is a few seconds, even for $N = 10$ on an SDS Sigma 7 computer.

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APPENDIX

The function $E_n(x)$ and related integrals

The exponential integral function $E_n(x)$ is defined as

$$E_n(x) = \int_0^\infty e^{-t} t^n \, dt = \sum_{n=1}^\infty e^{-n^2 x^2} \, dx.$$ (A1)

Since this function will be used many times in our calculations, we shall give a most efficient way of computing its values.
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\[ E_n(x) = \begin{cases} 
-\gamma \ln x + \sum_{i=1}^{\infty} a_i x^i, & 0 < x \leq 1, \\
\frac{e^{-x}}{\sum_{i=1}^{\infty} b_i x^i}, & 1 < x < \infty,
\end{cases} \]

where the coefficients are given by Abramowitz and Stegun. The above expression is accurate to \(1 \times 10^{-7}\) for all \(x\) and is adequate for our purpose. All of the other \(E_n(x)\) for \(n \geq 2\) are related to \(E_1(x)\) analytically. We may use the formula

\[ E_n(x) = \frac{1}{(n-1)!} \left[ (-x)^{n-1} E_1(x) + e^{-x} \sum_{i=0}^{n-2} (n-s-2)! (-x)^s \right]. \]

Thus, the evaluation of \(E_n(x)\) is easily accomplished. We define a few other useful integrals of \(E_n(x)\), namely

\[ l^* = \int_{\tau_1}^{\tau_{n+1}} \text{d} \tau E_n(\tau^* - \tau) = E_{n+1}(\tau^* - \tau_n) - E_{n+1}(\tau^* - \tau), \]

\[ y^*(\tau) = \int_{\tau_1}^{\tau_{n+1}} \text{d} \tau E_n(\tau - \tau) \]

\[ = \begin{cases} 
\frac{-\gamma}{n} E_{n+1}(\tau - \tau_n) - E_{n+1}(\tau_{n+1} - \tau) & \text{if } \tau < \tau_n < \tau_{n+1}, \\
E_{n+1}(\tau_n - \tau) - E_{n+1}(\tau_{n+1} - \tau) & \text{otherwise},
\end{cases} \]

\[ m^* = \int_{\tau_1}^{\tau_{n+1}} \text{d} \tau E_n(\tau - \tau) \]

\[ = \begin{cases} 
\frac{\gamma (\tau_{n+1} - \tau_n)}{n} - \frac{1}{n+1} + E_{n+1}(\tau_{n+1} - \tau) & \text{if } i = j, \\
E_{n+1}(\tau_n - \tau_j) + E_{n+1}(\tau_n - \tau_i) - E_{n+1}(\tau_n - \tau_j) & \text{if } i \neq j.
\end{cases} \]