QUADRATIC INTEGRALS IN INVERSE PROBLEMS WITH MULTIPLE SCATTERING

T. VIIK[1] AND N. J. MCCORMICK[2]
[1] *Tartu Observatory,*
Tõravere, Tartumaa, 61602, Estonia
[2] *University of Washington,*
Mechanical Engineering, Seattle, WA 98195-2600, USA

Abstract.

Procedures are described and tested for determining the single-scattering albedo using the measurement of specific intensities within or at the surfaces of homogeneous, finite or infinite atmospheres. Unpolarized radiation in an isotropically scattering semi-infinite atmosphere and polarized radiation in an atmosphere that scatters according to the Rayleigh-Cabannes law are considered. According to our numerical experiments the albedo of single scattering can be derived with great accuracy even when the measurements are not so accurate while the determination of other characteristics of the medium is much more complicated.

1. Introduction

It is well known that the equation of radiative transfer for a conservative medium has two exact integrals: the flux integral and the so-called K-integral which is closely connected with the radiative pressure. These integrals are linear with respect to the specific intensity. The transfer equation also admits quadratic integrals, first considered in detail by Rybicki [13] for a homogeneous semi-infinite atmosphere that scatters isotropically. He has shown that some of his integrals are related to the $\sqrt{\epsilon}$ - law (where ϵ is the probability of photon destruction in a single scattering event), a law much discussed in the literature (e.g., by Frisch and Frisch [5]).

Rybicki's quadratic integrals were generalized by Ivanov [6] in such a way that they relate the radiation fields at two different optical depths in an atmosphere. Ivanov showed that by using these integrals for determining the radiation field in an optically semi-infinite atmosphere the problem can be reduced to finding only the specific intensity for the downward radiation. He also noticed that one may obtain the quadratic integrals proceeding from completely different considerations [1].

Derivation and use of another type of quadratic integrals was initiated independently by Siewert in 1978 [15]. He showed how to determine the single-scattering albedo for unpolarized radiation in a semi-infinite atmosphere with isotropic scattering, and later extended the work to find the albedo and the coefficients for two-term [17] and three-term [18] phase functions for anisotropic scattering in optically finite or infinite atmospheres. For the two-term phase function no numbers were given, but according to some (unpublished) calculations by one of the authors (TV) the single-scattering albedo easily can be found, although the determination of the parameter of the phase function is extremely sensitive to errors in measuring the specific intensities. The errors in determining the numerical characteristics in the case of three-term phase function have been analyzed by Dunn and Maiorino [4].

McCormick developed two complementary sets of equations involving quadratic integrals for determining the albedo and an arbitrary number of scattering expansion coefficients, provided unpolarized intensity measurements are dependent on both the polar and azimuthal angles [7]. Numerical tests were performed by Oelund and McCormick [11] that demonstrated the sensitivity of the estimated parameters to simulated errors in the measurements, and provided insight into which of the two independent sets of equations was better.

For polarized radiation with a 2-vector intensity, Siewert [16] showed how to determine the single-scattering albedo from the measurements of the specific intensity of the emergent radiation from a Rayleigh-scattering half-space. Similarly, Siewert and Maiorino [19] exploited quadratic integrals to determine the single-scattering albedo λ and the albedo of a Lambertian bottom, λ_0, in a finite Rayleigh-scattering atmosphere, but the authors noted that accurate values of λ and λ_0 can be obtained only when exceptionally accurate experimental data become available.

Applying an approach similar to that of Siewert and Maiorino, McCormick [8] developed a procedure to determine the single-scattering albedo from polarization measurements of the specific intensity at two levels in a finite homogeneous atmosphere that scatters radiation according to the Rayleigh-Cabannes law with true absorption. Viik and McCormick [24] tested McCormick's procedure by solving the forward radiative transfer problem for the 2-vector specific intensity at two levels in the atmosphere or on its boundaries, [21]− [23] and then inducing random errors and trying to extract the single-scattering albedo and the depolarization factor.

In this report we demonstrate the similarity of the quadratic integrals for unpolarized radiation, as employed by Rybicki, to the quadratic integrals used by Siewert and McCormick for the 2-vector polarized radiation problem. We have assumed that both I- and Q-components may be measured to the same accuracy. This may not be the case, as pointed out by Mishchenko, [10] because the Q-component of the unpolarized incident flux is much smaller than I-component. How the difference in "measurement" errors influences the results remains to be studied in a forthcoming paper.

2. Rybicki's quadratic integrals for unpolarized radiation

To make the formulas more transparent we omit (where possible) the arguments of functions. We consider an atmosphere that is optically semi-infinite, homogeneous, and plane-parallel in which the radiation is scattered isotropically and monochromatically. Radiative transfer in such an atmosphere is described by

$$\mu \frac{\partial I}{\partial \tau} = I - S, \tag{1}$$

where $I(\tau, \mu)$ is the specific intensity at optical depth τ at an angle $\cos^{-1} \mu$ to the *negative* τ-axis. $S(\tau)$ is the source function

$$S = \lambda J + (1 - \lambda)B, \tag{2}$$

where λ is the albedo of single scattering, and

$$J = \frac{1}{2} \int_{-1}^{1} I(\tau, \mu) d\mu. \tag{3}$$

Next we define

$$I_+(\tau, \mu) \equiv I(\tau, \mu), \quad I_-(\tau, \mu) \equiv I(\tau, -\mu). \tag{4}$$

For these quantities

$$\mu \frac{\partial I_+}{\partial \tau} = I_+ - S, \quad -\mu \frac{\partial I_-}{\partial \tau} = I_- - S. \tag{5}$$

While

$$\frac{\partial}{\partial \tau}(I_+ I_-) = (S + \mu \frac{\partial I_+}{\partial \tau}) \frac{\partial I_-}{\partial \tau} + (S - \mu \frac{\partial I_-}{\partial \tau}) \frac{\partial I_+}{\partial \tau}, \tag{6}$$

we find that

$$\frac{\partial}{\partial \tau}(I_+ I_-) = S \frac{\partial}{\partial \tau}(I_+ + I_-). \tag{7}$$

From this equation Rybicki's quadratic integral $Q(\tau)$, defined by [13]

$$Q(\tau) = \frac{1}{2}\int_{-1}^{1} I(\tau,-\mu)I(\tau,\mu)d\mu, \tag{8}$$

is found to satisfy the equation

$$\frac{dQ}{d\tau} = 2S\frac{dJ}{d\tau}. \tag{9}$$

Rybicki also considered the quadratic integral

$$R(\tau) = \int_{-1}^{1} \mu^2 I(\tau,-\mu)I(\tau,\mu)d\mu. \tag{10}$$

Here this integral is considered only in the planetary problem. (In passing we note that these same two quadratic integrals were utilized by Siewert and McCormick for their applications.)

In the following we study only three kinds of internal sources: $B = 0$, corresponding to the Milne problem where the sources of radiation are deep in the atmosphere, the case with a constant source B, and the case with exponential sources in the planetary problem.

2.1. THE MILNE PROBLEM

For the Milne problem

$$\frac{dQ}{d\tau} = 2\lambda J\frac{dJ}{d\tau} = \lambda\frac{dJ^2}{d\tau}, \tag{11}$$

which can be integrated from τ_1 to τ_2 to give

$$Q(\tau_2) - Q(\tau_1) = \lambda\left[J^2(\tau_2) - J^2(\tau_1)\right]. \tag{12}$$

Because $Q(0) = 0$ it immediately follows that

$$\lambda = Q(\tau)\left[J^2(\tau) - J^2(0)\right]^{-1}. \tag{13}$$

This means that if we measure the specific intensities at optical depths $\tau > 0$ and $\tau = 0$ (preferably doing this at Legendre-Gauss nodes for better integrations) we find the single-scattering albedo.

2.2. THE CONSTANT SOURCE PROBLEM

Rybicki [13] also has shown that the Q-integral can be used for the case with a spatially homogeneous distribution of internal sources of radiation of magnitude B. This case represents a model of an isothermal atmosphere with B as the Planck function and, according to the Kirchhoff law, the internal source of radiative energy is proportional to ϵB, where ϵ is the probability of a photon's destruction in a single scattering event given by

$$\epsilon = 1 - \lambda. \tag{14}$$

With this definition we can rewrite Eq. (2) for the source function

$$S = (1 - \epsilon)J + \epsilon B. \tag{15}$$

After incorporating this equation into Eq. (9) it follows that

$$\frac{dQ}{d\tau} = (1 - \epsilon)\frac{dJ^2}{d\tau} + 2\epsilon B\frac{dJ}{d\tau}, \tag{16}$$

which immediately can be integrated to give

$$Q = (1 - \epsilon)J^2 + 2\epsilon BJ + \text{const.} \tag{17}$$

Rybicki went on to show, using the asymptotics at infinite optical depth, where $S = Q = J = B$, that

$$S^2(\tau) = (1 - \epsilon)Q(\tau) + \epsilon B^2. \tag{18}$$

At the outer boundary of an atmosphere, where $Q(0) = 0$ because there is no incoming radiation, the source function becomes

$$S(0) = \epsilon^{1/2}B, \tag{19}$$

which is called the $\sqrt{\epsilon}$-law for monochromatic scattering. Equation (18) is the generalization of this law to all optical depths in the atmosphere.

One may use either Eq. (18) or Eq. (19) for determining the destruction probability. Because it is easier to measure the intensities at the surface of an atmosphere, we use Eq. (19) for that purpose. After using Eq. (15) in Eq. (19) and remembering that all values are taken at $\tau = 0$ we get

$$(J - B)^2\epsilon^2 + (2JB - 2J^2 - B^2)\epsilon + J^2 = 0. \tag{20}$$

This quadratic equation can easily be solved for ϵ and its physically meaningful root is

$$\epsilon = \left(\frac{J}{J - B}\right)^2. \tag{21}$$

2.3. THE PLANETARY PROBLEM

Next we consider the planetary problem for a source function of the type

$$S = \lambda J + S^* \exp(-\tau/\mu_0), \tag{22}$$

where

$$S^* = \frac{1}{4}\lambda F \tag{23}$$

with πF the net flux of a parallel beam of radiation incident on a plane-parallel atmosphere per unit area normal to itself, and μ_0 is the direction cosine of the angle of incidence referred to the *outward* normal.

When generalizing the results by Rybicki [13] Ivanov [6] found an equation involving Q and R that can be evaluated for $\tau_1 = \tau_2 = \tau$ to give

$$S^2 = \lambda Q - \lambda R/\mu_0^2 + (1-\lambda)^{-1}\left[S^* + \lambda H/\mu_0\right]^2, \tag{24}$$

where

$$H = \frac{1}{2}\int_{-1}^{1} I(\tau,\mu)\mu d\mu. \tag{25}$$

For simplicity we consider here only the case $\tau = 0$ so that $Q = R = 0$. From Eq. (24) we have

$$\lambda = 1 - \left[\frac{4H + \mu_0 F}{\mu_0(4J + F)}\right]^2. \tag{26}$$

Thus, to determine the albedo of single scattering for the planetary problem one has to measure the mean intensity and the flux at the surface of the atmosphere.

3. Quadratic integrals and the inverse problem for polarized radiation

Next we consider the application of quadratic integrals for polarized radiation. We analyze an optically semi-infinite or finite homogeneous atmosphere that scatters radiation according to the azimuthally-averaged Rayleigh-Cabannes law for molecular scattering.

We consider two problems: the planetary problem with boundary conditions

$$\begin{aligned} \mathbf{I}(0,\mu) &= \mathbf{F}\delta(\mu-\mu_0), \quad 0 \le \mu \le 1, \\ \mathbf{I}(\tau_0,\mu) &= 0, \quad -1 \le \mu \le 0, \end{aligned} \tag{27}$$

for incident flux $\mathbf{F}$, and the Milne problem with a source deep in the interior, for which

$$\mathbf{I}(0,\mu) = 0, \quad 0 \le \mu \le 1, \tag{28}$$

and the intensity in deep layers does not increase more rapidly than $\exp(\tau)$. When dealing with the planetary problem we have to remember that in the following all the specific intensities of the downward radiation are sums of direct and diffuse components.

We proceed from the equation of transfer

$$\mu \frac{\partial}{\partial\tau}\mathbf{I}(\tau,\mu) + \mathbf{I}(\tau,\mu) = \frac{\lambda}{2}\mathbf{Q}(\mu)\int_{-1}^{1}\mathbf{Q}^T(\mu')\mathbf{I}(\tau,\mu')d\mu', \quad 0 \le \tau \le \tau_0, \tag{29}$$

where μ is measured from the *positive* axis of the optical depth τ and the intensity $\mathbf{I}$ is a 2-vector with components $I_\ell(\tau,\mu)$ and $I_r(\tau,\mu)$. The matrix $\mathbf{Q}(\mu)$ is defined as [2, 14]

$$\mathbf{Q}(\mu) = \frac{3}{2(c+2)^{1/2}}\begin{bmatrix} c\mu^2 + \frac{2}{3}(1-c) & (2c)^{1/2}(1-\mu^2) \\ \frac{1}{3}(c+2) & 0 \end{bmatrix}. \tag{30}$$

We first operate on Eq. (29) with the transpose vector $2\mathbf{I}^T(\tau,-\mu)$ and integrate over μ to obtain the scalar equation

$$2\int_{-1}^{1}\mathbf{I}^T(\tau,-\mu)\mu\frac{\partial}{\partial\tau}\mathbf{I}(\tau,\mu)d\mu = \lambda\mathbf{P}_0^T(\tau)\mathbf{P}_0(\tau) - S_0(\tau), \tag{31}$$

where

$$\mathbf{P}_n(\tau) = \int_{-1}^{1}\mu^n\mathbf{Q}^T(\mu)\mathbf{I}(\tau,\mu)d\mu \tag{32}$$

and

$$S_n(\tau) = 4\int_0^1 \mu^{2n}\mathbf{I}^T(\tau,-\mu)\mathbf{I}(\tau,\mu)d\mu. \tag{33}$$

After differentiating Eq. (31) and substituting Eq. (29) into Eq. (31) we get

$$-2\int_{-1}^{1}\mathbf{I}^T(\tau,-\mu)\frac{\partial}{\partial\tau}\mathbf{I}(\tau,\mu)d\mu + \lambda\mathbf{P}_0^T(\tau)\frac{d}{d\tau}\mathbf{P}_0(\tau) = \frac{d}{d\tau}\left[\lambda\mathbf{P}_0^T(\tau)\mathbf{P}_0(\tau) - S_0(\tau)\right]. \tag{34}$$

Next we add Eq. (34) and its transpose (with a reversal in the sign of μ) to obtain

$$\frac{d}{d\tau}\left[\lambda\mathbf{P}_0^T(\tau)\mathbf{P}_0(\tau) - S_0(\tau)\right] = 0. \tag{35}$$

This result immediately can be integrated over $\tau_1 \leq \tau \leq \tau_2$ to give

$$\lambda = [\mathbf{P}_0^T(\tau_1)\mathbf{P}_0(\tau_1) - \mathbf{P}_0^T(\tau_2)\mathbf{P}_0(\tau_2)]^{-1}[S_0(\tau_1) - S_0(\tau_2)]. \tag{36}$$

This is the equation involving the quadratic integral $S_0(\tau)$.

We can repeat the described procedure by operating on Eq. (29) with $2\mu\mathbf{I}^T(\tau, -\mu)$ and integrating over μ. Eventually we get [8]

$$\lambda[\mathbf{P}_1^T(\tau_1)(\mathbf{U} - \lambda\mathbf{R})^{-1}\mathbf{P}_1(\tau_1) - \mathbf{P}_1^T(\tau_2)(\mathbf{U} - \lambda\mathbf{R})^{-1}\mathbf{P}_1(\tau_2)] = S_1(\tau_1) - S_1(\tau_2), \tag{37}$$

where

$$(\mathbf{U} - \lambda\mathbf{R})^{-1} = \Delta^{-1} \begin{bmatrix} c + 2 - 12\lambda c/5 & \lambda(2c)^{1/2}(1 - 7c/10) \\ \lambda(2c)^{1/2}(1 - 7c/10) & c + 2 - \lambda(2 + 7c^2/10) \end{bmatrix} \tag{38}$$

for $\Delta = (1 - \lambda)(c + 2)(1 - 7\lambda c/10)$. Eq. (37) is an equation involving the second quadratic integral, $S_1(\tau)$.

4. Numerical tests

We performed numerical tests on the presented schemes by solving the respective forward radiative transfer problem and getting the specific intensities at the Gauss nodes. These results next were used as the mean values to which the normally distributed random errors

$$\varepsilon(x) = \delta \exp(-x^2/2\rho^2) \tag{39}$$

were added by sampling 10,000 "measurements." Here ρ is the dispersion of random errors of an individual measurement and δ is the amplitude of the error (i.e., $\delta = 0.1$ corresponds to an error magnitude of 10%).

To obtain the normally distributed pseudorandom errors we first used the RAN1 program [12] for getting uniformly distributed pseudorandom errors on (0,1). Then the Box-Muller method [12] was applied to transform these errors to normally distributed ones.

The direct problems for isotropic scattering were solved by applying the method of Viik *et al.* [20] and for polarized transfer by applying the method described in references 21-23.

In the following figures each line of mean values is bounded on either side by the values of the mean plus or minus two standard deviations. If there were no errors in specific intensities the curves would have been diagonal straight lines.

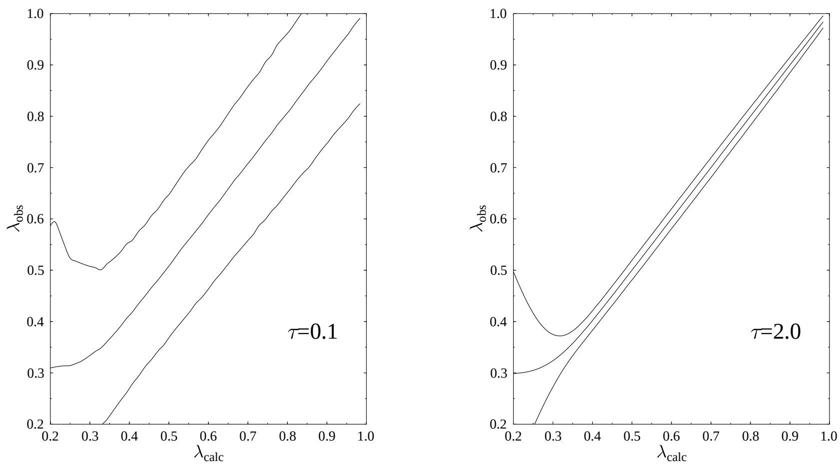

Figure 1. The Milne problem. λ_{obs} obtained from Eq. (13) versus λ_{calc} of forward problem for $\tau = 0.1$ and $\tau = 2.0$ with error amplitude $\delta = 0.05$ and individual dispersion $\rho = 1.0$.

4.1. THE MILNE PROBLEM

Determination of single-scattering albedos for this problem is very sensitive to "measurement" errors. Even for $\delta = 0$, with no errors at all, (consequently, the "measurements" were made to machine accuracy) we could not obtain good results even for small τ. However, in Fig. (1) we see that the accuracy was much better when $\lambda \to 1$ and the measurements were made deep inside the atmosphere. For example, if $\delta = 0.05$ we could obtain λ to an accuracy of 0.001 for $\lambda = 1$ and $\tau = 5.0$.

4.2. THE CONSTANT SOURCE PROBLEM

The calculations showed that the destruction probability (or the single-scattering albedo) can be obtained in a stable manner even for large error amplitudes of a single measurement ($\delta \leq 0.2$) if we only measure the specific intensity at the boundary of an atmosphere. Figure (2) shows how quickly this stability deteriorates if we try to transfer the measurements into the atmosphere according to Eq. (18). More-or-less trustworthy results can be obtained only for $\tau \leq 0.1$, which is understandable because for large optical

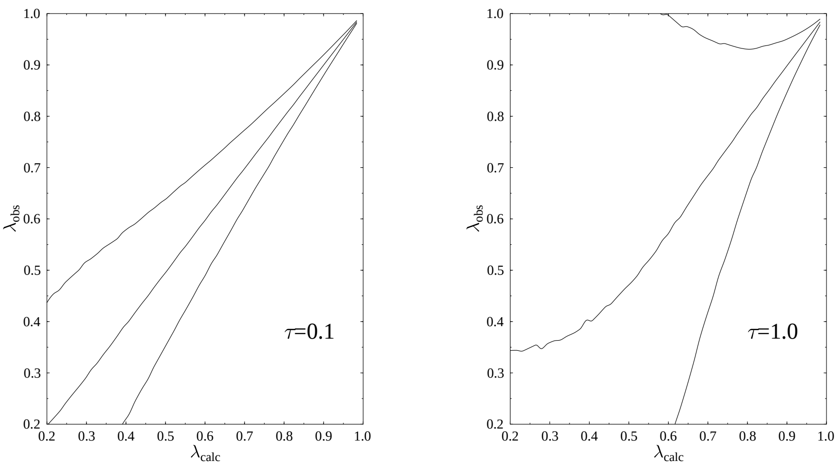

Figure 2. The constant source problem. $\lambda_{obs} = 1 - \epsilon_{obs}$ obtained from Eq. (21) versus λ_{calc} of forward problem for $\tau = 0.1$ and $\tau = 1.0$ with error amplitude $\delta = 0.10$ and individual dispersion $\rho = 1.0$.

depths the intensity I in the isothermal medium turns to B, independently of the destruction probability. If we want to determine ϵ from measurements in deeper layers we have to measure the specific intensity very accurately.

4.3. PLANETARY PROBLEM FOR POLARIZED RADIATION

Our calculations have shown that the single-scattering albedo can be obtained from Eq. (36) even if the error amplitude is $\delta \approx 0.25-0.3$. The results for λ in Fig. (3) with $\mu_0 = 0.5$ are very nearly the same as for $\mu_0 = 0.1$ reported earlier [24]. After having found λ from Eq. (36) we use it in Eq. (37) first to determine the number of possible values of the depolarization factor c. If there are two or three roots we have to use each c-value in our model to determine which minimizes the quadratic form

$$q = \int_{-1}^{1} [\mathbf{\Delta I}^T(\tau_2, \mu)\mathbf{\Delta I}(\tau_2, \mu) - \mathbf{\Delta I}^T(\tau_1, \mu)\mathbf{\Delta I}(\tau_1, \mu)] d\mu, \qquad (40)$$

where $\mathbf{\Delta I}(\tau, \mu)$ is the difference between measured values and those computed with the selected value of c.

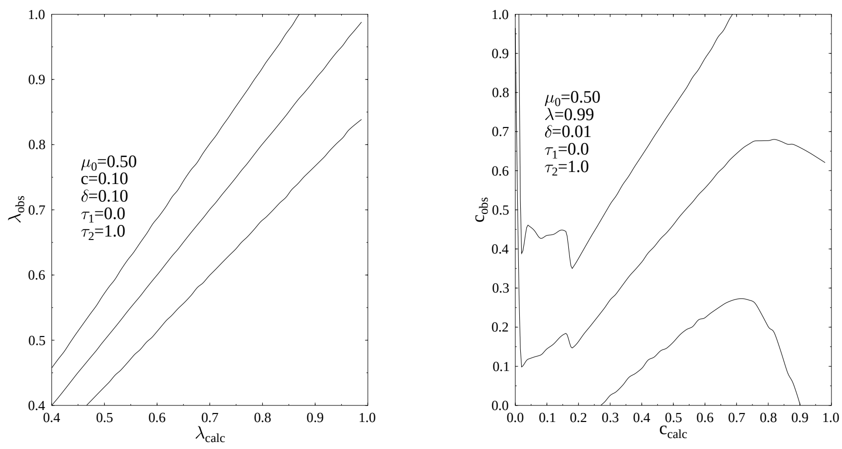

Figure 3. Molecular scattering. Left panel: λ_{obs} obtained from Eq. (36) versus λ_{calc} of forward problem for $c = 0.1$ with error amplitude $\delta = 0.1$. Right panel: c_{obs} obtained from Eq. (37) versus c_{calc} of forward problem for $\lambda = 0.99$ with error amplitude $\delta = 0.01$. For both figures the individual dispersion is $\rho = 1.0$ and planetary illumination is at $\mu_0 = 0.5$. The levels of "measurement" are $\tau_1 = 0.0$ and $\tau = 1.0$, respectively.

Here we demonstrate the influence of the two sets of parameters on the results of calculations. It is clear that even errors of only 1% in measured specific intensities may make the procedure unstable. The instabilities in determining c are very similar to those encountered by Siewert and Maiorino [19] when they considered a finite atmosphere with Lambertian reflection at the ground. They too found that λ could be determined more accurately than the Lambertian reflection coefficient.

5. Conclusions

As shown, the quadratic integrals Q and R of Rybicki for unpolarized radiation and the quadratic integrals S_0 and S_1 of Siewert and McCormick for polarized radiation are closely related. These integrals of radiative transfer provide us with a convenient tool for solving some elementary inverse problems. Numerical experiments have shown that for these problems the single-scattering albedo can be derived with great accuracy even when the measurements are not so accurate. The determination of other characteristics of the medium is much more complicated.

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References

1. D. Anderson, J. Inst. Maths. Applics. **12**, 55 (1973).
2. G.R. Bond, C.E. Siewert, Astrophys. J. **164**, 97 (1971).
3. S. Chandrasekhar: "Radiative Transfer" (Oxford University Press, 1950, [Dover, 1960]).
4. W.L. Dunn, J.R. Maiorino, J. Quant. Spectrosc. Rad. Transfer **24**, 203 (1980).
5. U. Frisch, H. Frisch, Mon. Not. Roy. Astron. Soc. **173**, 167 (1975).
6. V.V. Ivanov, Astronomicheskij J. **55**, 1072 (1978).
7. N.J. McCormick, J. Math. Phys. **20**, 1504 (1979).
8. N.J. McCormick, Astrophys. Space Sci. **71**, 235 (1980).
9. N.J. McCormick, R. Sanchez, J. Quant. Spectrosc. Rad. Transfer **30**, 527 (1983).
10. M.I. Mishchenko, private communication (2003).
11. J.C. Oelund, N.J. McCormick, J. Opt. Soc. Am. A **2**, 1972 (1985).
12. H.W. Press, B.P. Flannery, S.A. Teukolsky, T.W. Vetterling: "Numerical Recipes" (Cambridge University Press, 1986).
13. G.B. Rybicki, Astrophys. J. **213**, 165 (1976).
14. C.E. Siewert, E.E. Burniston, Astrophys. J. **174**, 629 (1972).
15. C.E. Siewert, J. Math. Phys. **19**, 1587 (1978).
16. C.E. Siewert, Astrophys. Space Sci. **60**, 237 (1979).
17. C.E. Siewert, J. Appl. Math. Phys. (ZAMP) **30**, 522 (1979).
18. C.E. Siewert, J. Quant. Spectrosc. Rad. Transfer **22**, 441 (1979).
19. C.E. Siewert, J.R. Maiorino, J. Appl. Math. Phys. (ZAMP) **31**, 767 (1980).
20. T. Viik, R. Rõõm, A. Heinlo, Tartu Teated **76**, 3 (1976).
21. T. Viik, Earth, Moon, and Planets **46**, 261 (1989).
22. T. Viik, Earth, Moon, and Planets **49**, 163 (1990).
23. T. Viik, J. Quant. Spectrosc. Rad. Transfer **66**, 581 (2000).
24. T. Viik, N.J. McCormick, J. Quant. Spectrosc. Rad. Transfer **78**, 235 (2002).

V. Ivanov and T. Viik (left) before the conquest of the Swallow's nest.