An adjoint formulation of the radiative transfer method

Qilong Min and Lee C. Harrison

Atmospheric Sciences Research Center, State University of New York at Albany, Albany

Abstract. Radiative transfer problems may be solved "adjointly" from an observed excident radiance flux distribution backward to the incident fluxes. We describe an adjoint formulation based on the discrete ordinate radiative transfer method, with application to atmospheric radiative transfer, including effects of the surface albedo. We compare this adjoint approach with forward radiative transfer solutions for a set of synthetic cases and also with observed surface irradiance data from a multifilter rotating shadow band radiometer (MFRSR). We compute the irradiances and mean intensities at arbitrary altitudes for fixed sky conditions but varying solar zenith angles. For these cases the adjoint method is comparably accurate and markedly faster.

Introduction

Radiative transfer computations are extremely time consuming. However, for certain applications where the forward approach is inefficient, one can employ an adjoint method for radiative transfer to reduce computational cost [Bell and Glasstone, 1970; Cacuci, 1981; Gerstl, 1982]. Unlike forward radiative transfer methods, which consider every photon, adjoint methods trace backward only those photons received by the observer or the response. In cases where many photons are scattered away from the observer adjoint methods may save significant computation time. In the sections that follow we compare forward and adjoint formulations of radiative transfer equations, the adjoint operator, boundary conditions, and applications of the adjoint method to three synthetic model atmospheres and to real surface radiance measurements from a rotating shadow band radiometer.

Adjoint Formulation of the Radiative Transfer Equation

The Forward Radiative Transfer Equation

The radiative transfer equations in plane parallel geometry may be written as follows:

$$-\mu \frac{dI^{dir}(z,\Omega)}{dz} = \beta^{ext} I^{dir}(z,\Omega)$$
(1a)
$$\mu \frac{dI^{dif}(z,\Omega)}{dz} = -\beta^{ext} I^{dif}(z,\Omega)$$
$$+ \frac{\beta^{sca}}{4\pi} \int_{4\pi} p(z,\Omega' \to \Omega) I^{dif}(z,\Omega) d\Omega'$$
$$+ \frac{\beta^{sca} F^{s}}{4\pi} p(z,\Omega_{0} \to \Omega) e^{-\tau/\mu_{0}}$$
(1b)

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Paper number 95JD03424. 0148-0227/96/95JD-03424\$05.00 with homogeneous boundary conditions, where $I^{dir}(z,\Omega)$ and $I^{dif}(z,\Omega)$ are the direct radiation and diffuse or scattered radiation, respectively. Both are a function of geometric altitude, z, cosine zenith angle, μ , direction, Ω , and the wavelength, λ . Here, $p(z,\Omega'\to\Omega)$ is a phase function from an incident solid angle, Ω' , into the excident angle, Ω . The last term in (1) is a pseudo-source of direct beam due to a parallel beam of sunlight with flux F^s normal to the beam direction $\theta_0 = \cos^{-1}\mu_0$. Also, $\beta^{ext} = \beta^{sca} + \beta^{abs}$, and β^{abs} , β^{sca} , and β^{ext} are the absorption, scattering, and extinction coefficients, respectively.

The direct radiation can be solved easily. Therefore we only discuss how to use the adjoint formulation of the radiative transfer problem, and a method of computational implementation to solve for scattered radiation. This equation may be written as $LI(z,\Omega) = Q(z,\Omega)$. L is an integral differential operator

$$L(z,\Omega) = \mu \frac{d}{dz} + \beta^{ext} - \frac{\beta^{sca}}{4\pi} \int_{4\pi} d\Omega' p(z,\Omega' \to \Omega) \eqno(2)$$

and $Q(z,\Omega)$ is a specified source.

The General Formulation of the Adjoint Method

In general, we consider a physical system governed by the equation

$$L(\rho)I(\rho) = Q(\rho) \tag{3}$$

with an appropriate boundary condition, where L is a linear operator, I is a distribution function, Q is a fixed source, and ρ represents all independent variables.

To obtain more accurate and efficient solutions of some integral property

$$G[I] = < \Sigma, I >$$

where brackets and angles represent functional relation and inner product, respectively, and Σ is the operator for a response function, we construct a variational principle for $G[I] = < \Sigma, I >$

$$F[I^*, I] = G[I] + \langle I^*, (Q - LI) \rangle$$

= $\langle \Sigma, I \rangle + \langle I^*, (Q - LI) \rangle$

where I^* is an arbitrary function to be defined below. The requirements that must be satisfied in order that Fbe a variational principle for G are as follows: (1) F is stationary about the function I which satisfies equation (3), and (2) the stationary value of F is $G[I] = \langle \Sigma, I \rangle$.

In the Hilbert space, the adjoint operator L^* is defined by

$$\langle I^*, LI \rangle = \langle L^*I^*, I \rangle \tag{4}$$

Therefore

$$\begin{split} \delta F &= < \Sigma, \delta I > + < I^*, \delta(Q - LI) > \\ &+ < \delta I^*, (Q - LI) > \\ &= < \Sigma, \delta I > - < L^*I^*, \delta I) > \\ &+ < \delta I^*, (Q - LI) > \\ &= 0 \end{split}$$

For arbitrary δI and δI^* leads to the requirement

$$LI = Q$$

$$L^*I^* = \Sigma$$
(5)

Clearly I satisfies equation (3). Equation (5) specifies the adjoint function I^* for a particular source Σ given a function of $G[I] = < \Sigma, I >$. Making use of (5), it is apparent that

$$F[I^*, I] = \langle \Sigma, I \rangle$$

= $\langle L^*I^*, I \rangle$
= $\langle I^*, LI \rangle$
= $\langle I^*, Q \rangle$ (6)

Thus F is a variational principle for $\langle \Sigma, I \rangle$. The advantage of an adjoint method to evaluate the integral property is demonstrated in (6). To calculate the radiative effects of m different sources, we must solve the forward radiative transfer equation m times. With the adjoint method, however, a radiative transfer equation set is solved only once, and the radiative effects of m different sources then require only m inner products.

Adjoint Operator for Radiative Transfer and **Boundary Conditions**

From (4) with appropriate boundary conditions to be discussed below, we may define the adjoint operator for the radiative transfer equation (e.g., equation (2)) as

$$L^{*}(z,\Omega) = -\mu \frac{d}{dz} + \beta^{ext}$$
$$-\frac{\beta^{sca}}{4\pi} \int_{4\pi} d\Omega' p(z, -\Omega' \to -\Omega) \quad (7)$$
$$= L(z, -\Omega)$$

We note that the forward and adjoint operators differ only in the sign of Ω . With this insight, the computation methods for the adjoint radiative equation can be developed by using the computation methods for the forward radiative transfer equation with some modifications. Now we consider the function

$$I'(z,\Omega) = I^*(z,-\Omega) \tag{8}$$

then

$$L^*(z,\Omega)I^*(z,\Omega) = L(z,-\Omega)I'(z,-\Omega) = \Sigma(z,\Omega)$$

Changing the variables from Ω to $-\Omega$, then

$$LI'(z,\Omega) = \Sigma(z,-\Omega)$$
 (9)

Thus we see that $I'(z,\Omega)$ is the forward radiance due to the source $\Sigma(z, -\Omega)$, and subject to appropriate boundary conditions. Hence to determine the adjoint radiance due to an adjoint source $\Sigma(z,\Omega)$, we first solve the forward radiative transfer equation for a "pseudosource" $\Sigma(z, -\Omega)$ to compute the "pseudo-radiance" I'. Finally, the adjoint radiance I^* is obtained from I' via (8).

The reflection from the lower boundary of the atmosphere, the surface of the Earth, is important in most atmospheric radiative transfer calculations. The solution to a Lambertian surface with albedo A can be constructed from the solutions to two standard problems with no ground reflection (vacuum boundary conditions) according to

$$I(z,\Omega) = I_{\nu}(z,\Omega) + F_{\nu}(0) \frac{A}{1 - A\hat{s}} I_{s}(z,\Omega)$$
 (10)

where I_v is the solution of standard problem for the given source, and $F_v(0)$ is the downward flux at the lower boundary. I_s is the solution to a problem of collimated illumination from the bottom,

$$LI_s = \mu U(\mu)\delta(z) \tag{11}$$

and

$$\hat{s} = \int_{o}^{2\pi} d\phi \int_{-1}^{0} d\mu \mid \mu \mid I_{s}(0, \Omega)$$
 (12)

where U is a step function and δ is the Dirac delta function [Liou, 1980]. Therefore we only need to discuss the boundary condition of adjoint radiance with respect to vacuum boundary conditions.

The vacuum boundary conditions for the forward radiance are

$$I(z_T, \mu, \phi) = 0$$
 for $-1 \le \mu < 0$ (13)
 $I(0, \mu, \phi) = 0$ for $0 < \mu \le 1$

where z_T denotes the altitude of the top of the atmosphere. Because the forward radiance must satisfy the $-\frac{\beta^{sca}}{4\pi}\int d\Omega' p(z,-\Omega'\to -\Omega) \quad (7) \quad \text{boundary conditions of (13), the requirement that both}$ the forward and adjoint radiances must satisfy (4) be-

$$\int_{o}^{2\pi} d\phi \int_{o}^{1} d\mu \mu I^{*}(z_{T}, \Omega) I(z_{T}, \Omega)$$

$$= \int_{o}^{2\pi} d\phi \int_{-1}^{0} d\mu \mu I^{*}(0, \Omega) I(0, \Omega)$$
(14)

Now $I(z,\Omega)$ and $I^*(z,\Omega)$ are both completely arbitrary and independent functions of z and μ . Thus the only way to ensure that (14) is satisfied is to require

$$I^*(z_T, \mu, \phi) = 0$$
 for $0 < \mu \le 1$ (15)
 $I^*(0, \mu, \phi) = 0$ for $-1 \le \mu < 0$

That is to say, it requires no outgoing adjoint radiance, in contrast with no incoming forward radiance.

In general, the forward radiative transfer method starts with a stream of photons and traces their progress through a scattering-absorptive medium. An observer looking backward through the medium does not detect the photons that are absorbed, or those that are scattered beyond his instrumental acceptance angle, so that he may not be able to use information carried by these "lost" photons to deduce the properties of the scattering medium. This means that much of the effort expended in tracing these photons is wasted. For such cases adjoint radiative transfer methods, which trace the arriving photons backward through the medium, may have computational economies and comparable numerical accuracy.

One common case where this occurs is the computation of surface-based solar irradiance as a function of solar zenith angle. In this case, and generally when the number of input parameters (or sources) exceeds the number of different responses of interest, adjoint methods are significantly more efficient than the traditional forward approach.

Application of the Adjoint Formulation of a Discrete Ordinate Method

Radiative transfer problems can be solved with a variety of techniques [Stamnes, 1986]. We adopt a discrete ordinate method as efficient and reliable [Stamnes et al., 1988]. The implementation includes all orders of multiple scattering and is valid for vertically inhomogeneous, nonisothermal, plane-parallel media. The atmosphere is divided into a series of homogeneous layers in which the scattering and absorbing properties are taken to be constant within each layer, but allowed to vary from layer to layer.

By appealing to the reciprocity principle, Stamnes [1982] showed that the boundary irradiance for collimated beam illumination is proportional to the exit angular intensity for uniform illumination. Thus by applying a uniform illumination to the top of the slab (and also from the bottom if it is vertically inhomogeneous), one may obtain boundary irradiance from all

desired solar zenith angles. However, it does not appear possible to compute irradiance or mean intensity at arbitrary altitudes. Here we consider specifically the adjoint method for solving the downward irradiance at an arbitrary altitude. Other problems may be handled in an analogous manner. The response function of the downward diffuse flux at altitude of z_0 , that is, adjoint source Σ , is

$$\Sigma = \mid \mu \mid \delta(z - z_0)U(-\mu) \tag{16}$$

The adjoint problem may then be solved using the angle-reversing procedures derived in the last section,

$$LI' = \mu U(\mu)\delta(z - z_0)$$

$$I'(z_T, \mu, \phi) = 0 \quad \text{for} \quad -1 \le \mu < 0 \quad (17)$$

$$I'(0, \mu, \phi) = 0 \quad \text{for} \quad 0 < \mu \le 1$$

This is a standard radiative transfer equation with no ground reflection, and it is apparently identical to (11) when z_0 is zero. However, the "pseudo-source" in this equation is an anisotropic source, which requires us to modify the standard methods to handle an arbitrary anisotropic source [Min et al., 1993]. Solving (17), we can evaluate the downward flux, $F_d(z_0)$, for any given surface albedo and solar zenith angle via (6), (8), and (10) as

$$F_d(z_0) = \langle I^*(z,\Omega), \frac{\beta^{sca}F^s}{4\pi}p(z,\Omega_0 \to \Omega)e^{-\tau/\mu_0} \rangle$$
(18)

In the future we hope to present a perturbation technique based on the adjoint formulation, which provides accurate estimates of radiative effects $(L+\delta L)$ as well as the derivatives of radiative properties for climate modeling and remote sensing, once the value of the effect is known for a "similar" model atmosphere (L).

Tests of Synthetic Cases

To validate our adjoint method, we compared the downward diffuse fluxes $(w\,m^{-2}\,nm^{-1})$ and the mean intensities at multiple altitudes calculated by both forward and adjoint methods for six synthetic cases. All the calculations, except the fifth case, were computed with four streams.

Case 1, a cloud free sky, was tested by adopting the midlatitude winter model of Air Force Geophysics Laboratory (AFGL) as the atmospheric gases [Anderson et al., 1986] and the aerosol model from MODTRAN 2 [Berk et al., 1989]. Figure 1 shows the downward diffuse fluxes calculated by the forward and adjoint at 415 nm for solar zenith angle from 0° to 80° at altitudes of 0, 1, 5, and 10 km. The background fall-winter aerosol was specified to give a visibility of 50 km, and the surface albedo was assumed to be 0.5. The differences between two methods are less than 0.08%, too small to be distinguished in the upper panel of Figure 1.

Case 2 considered water droplet clouds at three optical depths. The optical properties of water cloud are

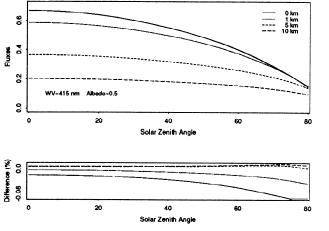


Figure 1. Case 1: Calculated downward fluxes at 415 nm at different altitudes from 0° to 80° solar zenith angles by using the adjoint and forward methods for the aerosols with the surface albedo of 0.5, and the differences between two methods.

adopted from Hu and Stamnes [1993]. Figure 2 shows the comparison between two methods at a wavelength of 415 nm for a water cloud layer inserted between 1 and 2 km with different optical depths of 0.3, 3, and 30, representing a thin cloud, moderate cloud, and thick cloud, respectively. The optical depths of cloud were obtained by assuming an effective droplet radius of 10 μ m and adjusting the liquid water content of the cloud. These comparisons have been carried for solar zenith angles from 0° to 80°, with a Lambertian surface albedo of 0.5. The adjoint method shows accuracy comparable to that of the forward method: both results are indistinguishable in Figure 2 (upper panel), and the differences between two methods are less than 0.08 % (lower panel).

Case 3 compared the results from both methods at 500 nm with a cirrus cloud layer between 11 and 12 km at three different altitudes: at the surface, below

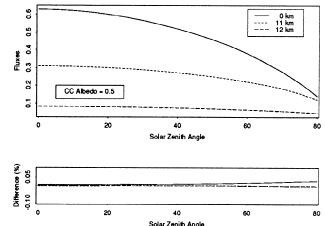


Figure 3. Case 3: Calculated downward fluxes at 500 nm at three different altitudes from 0° to 80° solar zenith angles by using the adjoint and forward methods for the cirrus cloud with the surface albedo of 0.5 and the differences between two methods.

the cloud, and above the cloud. The optical properties of cirrus cloud are adopted from MODTRAN 2 [Berk et al., 1989]. The results, shown in Figure 3, again illustrate very small differences.

Case 4 tested the accuracy of our adjoint method by varying the surface albedo: 0.1, 0.5, and 0.9. The downward diffuse fluxes at 415 nm were computed by using both methods with a moderate cloud layer that was placed between 1 and 2 km with a optical depth of 3, shown in Figure 4. As the optical depth increases the scattered irradiance is increasingly sensitive to the surface albedo. The higher surface albedo results in a larger downward diffuse flux. These comparisons demonstrate that the adjoint method agrees very well with the forward method for large surface albedos.

Further, in case 5, we tested our model varying the number of streams. The downward fluxes at 500 nm

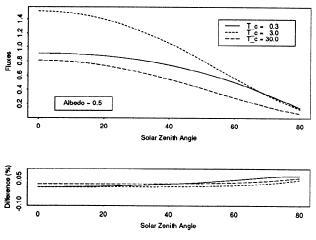


Figure 2. Case 2: Calculated downward fluxes at 415 nm from 0° to 80° solar zenith angles by using the adjoint and forward methods for three water cloud cases with different optical depths: 0.3, 3.0, and 30, and the differences between two methods.

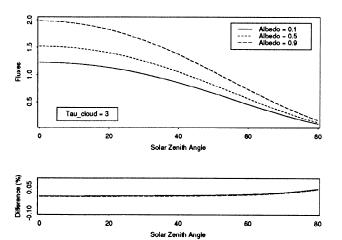


Figure 4. Case 4: Calculated downward fluxes at 415 nm from 0° to 80° solar zenith angles by using the adjoint method and forward method and the differences for the water cloud cases with three different surface albedos: 0.1, 0.5 and 0.9.

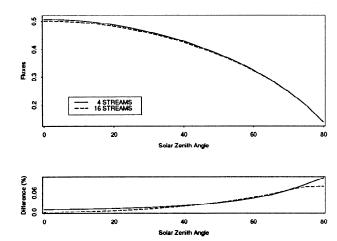


Figure 5. Case 5: Calculated downward fluxes at 500 nm and comparisons between the adjoint method and forward method for different streams: 4 and 16 from 0° to 80° solar zenith angles.

have been calculated by using both forward and adjoint methods with 4 and 16 streams for a clear sky case. In these cases, a surface albedo of 0.5 was assumed. The adjoint method agrees very well with the forward method, as shown in Figure 5. The difference is less than 0.1% for these cases. Figure 5 also illustrates that the accuracy of the adjoint method is equal to that of the forward method, because the adjoint radiance is computed by using the angle-reversing procedure of the forward method.

The mean intensity or "actinic flux" is the quantity of interest when calculating photolysis rates and UV doses. There is a need for fast computation of these quantities in photochemical modeling and also in the biological community concerned with UV dose assessments. Finally, in case 6, we applied our adjoint method to evaluate the mean intensity and compared with the forward

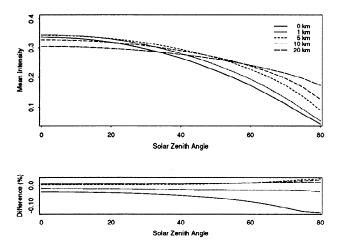


Figure 6. Case 6: Calculated mean intensities at 415 nm and comparisons between the adjoint method and forward method for five different altitudes: 0, 1, 5, 10, and 20 km from 0° to 80° solar zenith angles.

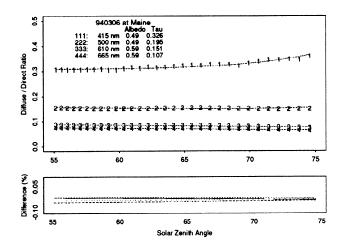


Figure 7. (top) Measured and calculated fluxes at 415, 500, 610, and 665 nm from 55° to 75° solar zenith angle: numbers of 1, 2, 3, and 4 representing the observed data for wavelengths at 415, 500, 610, and 665, respectively; solid line representing the results by the forward method; dotted line representing the results by the adjoint method. (bottom) The differences between the forward and adjoint methods.

method for five altitudes: 0, 1, 5, 10, 20 km. The adjoint source for an arbitrary altitude is $\Sigma = \delta(z - z_0)$. Solving the adjoint radiative equation once, we can compute the mean intensity for all desired solar zenith angles at altitude z_0 by taking inner products. The atmospheric conditions in this case is the same as discussed in case 1. The accuracy of the adjoint method has illustrated in Figure 6. The differences between two methods are less than 0.15% everywhere.

Comparison Against Real Measurements

A multiple filter rotating shadow band radiometer (MFRSR), developed by Harrison et al. [1994], permits a single sensor at each wavelength to acquire the total horizontal, diffuse horizontal, and direct normal spectral irradiance. This geometry guarantees that the calibration coefficients are identical for each irradiance component, which eliminates the uncertainty associated with intercomparisons of solar component measurements made with separate sensors. The direct and diffuse components contain all the information about the atmospheric effects, as they penetrate through the atmosphere. Therefore this ratio is insensitive to the calibration error, but it depends sensitively upon such interesting characteristics as atmospheric aerosol loading, ground albedo, sky cover, and the vertical distribution of ozone [Chai and Green, 1976; King and Herman, 1979; Frederick et al., 1989; Zeng et al., 1994], and also provides a method of evaluating model performance.

Finally, we computed the downward diffuse to direct ratio by using both forward and adjoint methods and compared those with the measurements of the MFRSR at the Maine Quantitative Links site. We chose clear

sky data in the afternoon of March 6, 1994, with solar zenith angles from 55° to 75°, eliminating the large early morning variations associated with relative humidity effects on aerosol scattering. Larger solar zenith angles were avoided because our one-dimensional plane parallel radiative transfer model does not account for a spherical Earth. Figure 7 shows the measurements of the MFRSR and the results of the forward and adjoint calculations for the four channels of 415, 500, 610, and 665 nm. The total optical depths were inferred from direct normal irradiance by Langley regression 0.326, 0.195, 0.151, and 0.107 for the channels of 415. 500, 610, 665 nm, respectively [Harrison and Michalsky, 1994]. The ground was covered with snow; surface albedos were assumed to be 0.49 for 415 and 500 nm, and 0.59 for 610 and 665 nm, to yield a best agreement with the measurements. Despite small fluctuations in the observed diffuse to direct ratio, which may be due to sparse clouds or to horizontal inhomogeneities in the atmospheric aerosols, the diffuse to direct ratios calculated by both forward and adjoint methods agree well with the measurements, and the differences between the two methods are less than 0.05 % everywhere.

The computational time of the forward method is much longer than that of the adjoint method, depending on the number data points, that is, computational timescales linearly with the number of solar zenith angles considered. For this case with 31 data points, the computational time of the forward method is about 31 times longer than that of the adjoint method.

Summary

In this paper we have described an adjoint discrete ordinate method for radiative transfer computations through vertically inhomogeneous atmospheres, and have demonstrated its speed and accuracy upon synthetic data, and with measurements by a multifilter rotating shadow band radiometer. The advantage of the adjoint method of radiative transfer is reduced computing time in certain applications, such as evaluating the mean intensity and irradiance profiles for varying solar zenith angles. It allows us to improve the photochemical modeling, and to invert the optical properties of the atmosphere from the ground observations, or from the satellite remote sensing, in a more rigorous manner.

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Qilong Min and Lee C. Harrison, Atmospheric Sciences Research Center, State University of New York at Albany, 100 Fuller Road, Albany, NY 12205. (e-mail: min@solsun1.asrc.albany.edu; lee@solsun1.asrc.albany.edu)

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