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Application of the Adjoint Method in Atmospheric Radiative Transfer Calculations

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ABSTRACT

The transfer of solar radiation through a standard mid-latitude summer atmosphere including different amounts of aerosols (from clear to hazy) has been computed. The discrete-ordinates (S_N) method, which has been developed to a high degree of computational efficiency and accuracy primarily for nuclear radiation shielding applications, is employed in a forward as well as adjoint mode. In the adjoint mode the result of a transfer calculation is an importance function (adjoint intensity) which allows the calculation of transmitted fluxes, or other radiative responses, for any arbitrary source distribution. The theory of the adjoint method is outlined in detail and physical interpretations are developed for the adjoint intensity. If, for example, the downward directed solar flux at ground level, $F_\lambda(z=0)$, is desired for N different solar zenith angles, a regular (forward) radiative transfer calculation must be repeated for each solar zenith angle. In contrast, only 1 adjoint transfer calculation gives $F_\lambda(z=0)$ for all solar zenith angles in a hazy aerosol atmosphere, for 1 wavelength interval, in 2.5 seconds on a CDC-7600 computer. A total of 155 altitude zones were employed between 0 and 70 km, and the convergence criterion for the ratio of fluxes from successive iterations was set at 2×10^{-3}. Our results demonstrate not only the applicability of the highly efficient modern S_N codes, but indicate also conceptual and computational advantages when the adjoint formulation of the radiative transfer equation is used.

I. Introduction

The transfer of both solar and terrestrial infrared radiation through the atmosphere can be described mathematically by the well-known radiative transfer equation[1] which is a special form of the linear Boltzmann equation [2] governing the transport of any neutral particles through a given medium. Particularly in nuclear technology, the linear Boltzmann equation* is the basis for the calculation of neutron and gamma radiation fields due to nuclear radiation sources such as radioactive materials or reactor cores. Due to the importance of an accurate prediction of neutron and gamma ray distributions around nuclear reactors for radiation shielding purposes, a large amount of research and development has been invested during the last 35 years to solve the linear Boltzmann equation efficiently for almost any prespecified degree of accuracy. These R & D investments have resulted in many diversified computational methods such as semi-empirical, spherical harmonics, discrete ordinates, and Monte Carlo methods. Advantages and disadvantages of these different calculational tools are discussed elsewhere[2].

In contrast, methods developed to solve solar and infrared radiative transfer problems in the atmosphere for meteorology or climatology applications have centered mostly around semi-empirical methods for broad-based overview calculations[3,4] and the spherical harmonics method for high-resolution detail analyses[5,6]. Other methods like the doubling method[7] and the method of successive orders of scattering[8] are also developed to a high degree of sophistication and computer effectiveness. Since the linear Boltzmann equation also describes problems in atmospheric radiative transfer, it is evident therefore that the computational

*also often called the transport equation.

methods developed primarily for nuclear radiation transport calculations, also must be applicable to solar and infared radiative transfer problems. We attempt to demonstr in this paper that the highly-developed discrete-ordinates (S_N) method may be used advantageously for meteorology or climatology applications. In addition, since most S_N codes are capable of solving the linear Boltzmann equation both in a forward as well as an adjoint mode, we shall also demonstrate how an adjoint solution may offer additional benefits in certain cases.

The discrete ordinates method, as developed by Chandrasekhar, has been successfully applied before to atmospheric radiative transfer problems by Liou[9]. However, Liou developed his own special-purpose code to solve the S_N equations in which he could not take full advantage of many recently developed numerical techniques such as special differencing methods or iterative acceleration methods. Hence, although Liou could demonstrate the principle applicability and accuracy of S_N methods, a comparison with other methods cannot yield any general conclusion about the computational effectiveness of S_N methods. In contrast, we are applying an off-the-shelve S_N code which incorporates today's state-of-the-art numerical techniques so that a computer time comparison with other standard codes may allow a more general conclusion. We will not describe any details pertaining to the S_N method itself nor the code since both are well-documented elsewhere [10,11]. We will concentrate instead on developing the mathematical basis for the adjoint method and the physical interpretation of the adjoint intensity in order to lay the groundwork for a deeper understanding of possible advantages in using the adjoint method.

II. Theory

The basic radiative transfer (or linear Boltzmann) equation for monochromatic radiation in a plane-parallel atmosphere may be written as[1,2]

$$-\mu \frac{\partial I}{\partial x} + \Sigma_t(x)I - \int_{-1}^{+1} d\mu' \int_0^{2\pi} d\phi' \Sigma_s(x;\mu'\rightarrow\mu,\phi'\rightarrow\phi)I(x,\mu',\phi') = Q(x,\mu,\phi) \qquad (1)$$

where $I(x,\mu,\phi)$ is the intensity distribution at level x in direction μ,ϕ, and $Q(x,\mu,\phi)$ denotes an arbitrary radiation source distribution. For a solar radiative transfer problem the spatial variable x may be measured as the distance from the top of the atmosphere vertically down while the direction variables μl and ϕ are measured with respect to the upward normal vector. Σ_s and Σ_t denote the scattering and total (scattering plus absorption) cross-sections for the atmosphere, respectively, which are assumed to be given for any x. The often-used scattering phase function is defined as $P = 4\pi\Sigma_s/\Sigma_t$.

If only solar radiation is considered, then the source distribution Q may be written as

$$Q(x,\mu,\phi) = \tfrac{1}{4}F_0\delta(x)\delta(\mu+\mu_0)\delta(\phi-\phi_0) \quad , \qquad (2)$$

where πF_0 is the incident solar flux at x=0, and $-\mu_0$, ϕ_0 identify the incident direction for the monodirectional solar flux. In general, the objective of a radiative transfer calculation is the computation of an integral response such as a netradiation flux in the upward or downward direction, a total transmission or reflection (albedo) at a certain altitude, a photodissociation or absorption rate, etc. All such radiative responses may be computed as a phase-space integral of the form

$$\text{Response} = \int_0^{\infty} \int_{-1}^{+1} \int_0^{2\pi} R(x,\mu,\phi)I(x,\mu,\phi)dxd\mu d\phi \quad , \qquad (3)$$

where R is a given response function and I the solution of Eq. (1). If, for example, the downward directed solar radiation flux* at the ground level $x=\tau$ (altitude zero) is desired, then Eq. (3) takes the form

$$F{\downarrow}(\tau) = \int_{-1}^{0} \int_{0}^{2\pi} \mu \, I(\tau,\mu,\phi) d\mu d\phi \ . \tag{4}$$

Comparing Eq. (4) with Eq. (3) we note that R in this case is chosen as

$$R(x,\mu,\phi) = \mu\cdot\delta(x-\tau)\theta(-\mu) \quad , \tag{5}$$

where $\theta(\mu)$ is the well-known Heavyside step function which is 1 for $\mu>0$ and zero for $\mu<0$.

In order to derive the adjoint transfer equation we introduce a simplifying operator notation and rewrite Eq. (1) as

$$L \ I = Q \quad , \tag{1a}$$

where L is called the linear Boltzmann operator. The phase-space integral in Eq. (3) is abbreviated as an inner product by brackets:

$$\text{Response} = \langle R,I \rangle \quad . \tag{3a}$$

The theory of linear operators [12] defines now an associated operator to L which is denoted L^+ and called the adjoint operator to L. L^+ is uniquely defined if for any two arbitrary functions I and I^+ the following commutation relation holds:

$$\langle I^+, LI \rangle = \langle I, L^+ I^+ \rangle \quad . \tag{6}$$

Specifically, the adjoint to the linear Boltzmann operator defined by Eqs. (1) and (1a) is

$$L^+ = +\mu \frac{\partial}{\partial x} + \Sigma_t(x) - \int_{-1}^{+1} d\mu' \int_{0}^{2\pi} d\phi' \Sigma_s(x;\mu\to\mu';\phi\to\phi') \quad , \tag{7}$$

which differs from L only by the sign in the first (streaming) term and

*In nuclear terminology a flux expressed by Eq. (4) is called a current.

an interchange of initial and final directions in the scattering integral term. The function $I^{+}(x,\mu,\phi)$ is called the adjoint function to $I(x,\mu,\phi)$ if it is chosen as the solution of the adjoint radiative transfer equation

$$L^{+}I^{+} = R \quad , \tag{8}$$

where the arbitrary response function R is taken as the adjoint source term.

The physical meaning of the adjoint intensity distribution I^{+} and the potential usefulness of Eq. (8) can be shown as follows: Multiplying Eq. (1a) by I^{+} and integrating over all phase space yields $\langle I^{+},LI\rangle = \langle I^{+},Q\rangle$, while multiplying Eq. (8) with I and integrating gives $\langle I,L^{+}I^{+}\rangle = \langle I,R\rangle$. Due to the defining commutation relation for L^{+}, Eq. (6), the left-hand sides of the above two equations are equal from which follows that

$$\langle I^{+},Q\rangle = \langle I,R\rangle \quad . \tag{9}$$

The right-hand side of Eq. (9) is recognized as the typical integral response, Eqs. (3) and (3a), which is the goal of any radiatvie transfer calculation. The left-hand side of Eq. (9) identifies therefore a second recipe to calculate such integral responses by using the adjoint intensity I^{+}. Remember, that Eq. (9) was derived for any arbitrary functions Q and R. For the sake of physical interpretation, let us chose R according to Eq. (5) which yields the as integral response the downward flux at groundlevel, $F\downarrow(\tau)$, according to Eq. (4). As a special radiation source distribution we assume a delta-function source in phase space, $Q_{0} = \delta(x-x_{0})\delta(\mu-\mu_{0})\delta(\phi-\phi_{0})$. Then all integrations in Eq. (9) can be carried out and we obtain

$$I^{+}(x_{0},\mu_{0},\phi_{0}) = F_{0}\downarrow(\tau) \quad . \tag{10}$$

In other words, the adjoint intensity at the phase space point (x_{0},μ_{0},ϕ_{0})

can be interpreted as that contribution to the downward flux $F_o{\downarrow}(\tau)$ at groundlevel which is due to a photon that was born at level x_o in direction μ_o, ϕ_o. Therefore the adjoint function I^+ is also called an importance function [13] with respect to the detector response defined by R.

Returning again to the transfer problem where the solar radiation is specified as a source distribution according to Eq. (2) the left-hand side of Eq. (9) can then also be integrated for this choice of Q and gives

$$\langle I,R \rangle = \tfrac{1}{4}F_o I^+(0,-\mu_o,\phi_o) \quad . \tag{11}$$

Eq. (11) indicates that any desired integral response $\langle I,R \rangle$ is given directly by the adjoint intensity at the top of the atmosphere (x=0) and for the direction of the incident solar radiation $-\mu_o,\phi_o$. To obtain this specific value of the adjoint intensity, the adjoint transfer equation, Eq. (8), needs to be solved with the appropriate response function R as an adjoint source. If, as in the following sample calculation, the radiative response of interest is chosen to be the downward flux at ground level, Eq. (4), then the adjoint transfer equation must be solved with an adjoint source term R according to Eq. (5). In this case then Eq. (11) reduces to

$$F{\downarrow}(\tau) = \tfrac{1}{4}F_o \; I^+(0,-\mu_o,\phi_o) \quad . \tag{12}$$

Comparing now Eq. (12) with the conventional recipe to compute $F{\downarrow}(\tau)$, namely Eq. (4), it might be suspected that in certain cases the use of Eq. (12) may be advantageous over the use of Eq. (4). Both formulas require the solution of a radiative transfer equation, namely either the "forward" transfer equation, Eq. (1), to obtain I, or the adjoint transfer equation, Eq. (8), to obtain I^+. Only the specific problem characteristics, i.e. the form of Q and R, determine which of the two mathematically equivalent formulations may be advantageous. The following sample calculation demonstrates clearly one practical case where the adjoint method offers substantial conceptual and computational advantages.

III. A Sample Application of the Adjoint Method to Compute the Diurnal Variation of Solar Irradiance.

Consider the classical problem of the transfer of solar radiation through the atmosphere where the integral response of interest is the downward directed total flux at ground level as a function of the solar zenith angle. The standard procedure for the solution of this problem is to solve the transfer equation, Eq. (1), for a number of different source terms Q_n, n=1,...,N, which are chosen so that each Q_n represents a different solar zenith angle $\mu_o^{(n)}$. This leads to a set of N different solutions of Eq. (1), say I_n, which, through Eq. (4), gives then the desired result in the form of a series $F{\downarrow}_n(\tau)$ for N different solar zenith angles.

In contrast, however, employing the adjoint method requires the solution of the adjoint transfer equation, Eq. (8), with the adjoint source term R chosen according to Eq. (5). The solution, namely the adjoint intensity distribution $I^+(x,\mu,\phi)$, contains immediately the solution to our transfer problem, according to Eq. (12). Ideally the adjoint intensity at the top of the atmosphere, $I^+(0,\mu,\phi)$, may be obtained for all directions μ,ϕ, which, for negative zenith angles $\mu = -\mu_o$ includes $I(0,-\mu_o,\phi_o)$ for all solar zenith angles μ_o and all solar azimuth angles ϕ_o. The factor $\frac{1}{4}F_o$ in Eq. (12) provides only the proper normalization of the adjoint solution to the solar source strength.

Figure 1 compares schematically the regular ("forward") and adjoint solution methods as discussed above. For the spatial variable in Fig. 1 the altitude z is chosen, as opposed to the distance x from the top of the atmosphere which is used throughout all equations in the text. The transformation for x to z is straightforward via $x = \tau - z$.

A numerical analysis has also been performed for this sample problem, using the one-dimensional discrete-ordinates code ONETRAN[11]. This code has been developed primarily for reactor physics and shielding applications where usually the transport of neutrons and gamma rays through structural and other materials is of concern. However, like almost all neutron transport codes, ONETRAN has a built-in adjoint capability. Therefore we can use this code to solve our solar radiation transfer problem in both the forward and adjoint modes. For simplicity we performed the calculations only for one wavelength, λ=0.6954 μm, which corresponds to a ruby laser frequency for which atmospheric cross-section data are easily obtained from the literature. Macroscopic molecular absorption and scattering cross-sections for a standard midlatitude summer atmosphere were taken from McClatchey et. al.[14] who give these data for 32 altitude layers from zero to 70 km altitude. The latter was chosen as the top of the atmosphere. In order to compare our results with other published data, we normalized the incident solar source strength to unity, i.e. the factor $\frac{1}{4}F_o$ in Eq. (2) and consequently also in Eq. (12) was set to 1.0. In this case the quantity $F\downarrow(\tau)$ can also be interpreted as the total transmission of the atmosphere for the given wavelength.

Fig. 2 summarizes the results from our calculations. In all cases the numerical values for the total transmission for a given solar zenith angle were identical within the accuracy set by the convergence criteria when calculated independently by the forward and adjoint methods, as described before. In addition, for the case without aerosols, our results could be directly compared to earlier reference calculations by Liou[9]. Both are in good agreement. Since McClatchy et. al.[14] give also cross-sections for two types of aerosols, "clear" for 2[illegible] ground visibility V_o, and "hazy" for V_o=5 km, we added to Fig. 2 also the solutions for these two polluted atmospheres. The specific solar zenith angles $\zeta_{1,2,4,7}$ indicated on the abscissa in Fig. 2 by arrows, correspond to four discrete directions as explicitly contained in the S_8 Gauss-Legendre angular quadrature set [11] used in our ONETRAN calculations. It should be noted again, that in order to obtain each one of the curves in Fig. 2 by means of the standard forward solution method, it is necessary to run ONETRAN for a series of different solar zenith angles and then interpolate the results. In contrast, the adjoint method requires only one single adjoint ONETRAN run to obtain each of the three curves because, according to Eq. (12) with $\frac{1}{4}F_o$=1.0, the total transmission is given directly by the adjoint intensity distribution at the top of the atmosphere as a function of zenith angle.

Table 1 gives a very simplified computer time comparision between the CPU-time (central processor unit time) needed for our calculations and that given for a comparable calculation using another solution technique. Luther[15] reported such a calculation using the successive-scattering iterative procedure of Davé and Gazdag[16] where 500 horizontal atmospheric layers were used and 91 discrete values of μ_i were employed. Using a convergence criterion of 1.002 (maximum allowed fraction $I_{m+1}(\tau,\mu_i)/I_m(\tau,\mu_i)$ for all μ_i and iteration index m) Luther[15] quotes a typical running time of about 20 minutes on a CDC-7600 for a full solar spectrum calculation. Since 83 discrete spectral intervals were employed we estimate an average running time of 14.6 seconds per interval. Our computations with ONETRAN have been performed with comparable detail resolution (80 discrete angles, 155 altitude zones, convergence within 1.002 for all pointwise intensities) with a typical CDC-7600 running time of 2.4 seconds for one wavelength. Since the adjoint of the Boltzmann operator is mathematically very similar to the (forward) Boltzmann operator itself (compare Eqs. (1) and (7)), an adjoint ONETRAN run requires roughly the same computer time as a forward run with otherwise the same parameters. No attempt has been made in our calculations to minimize the computer time in any way, and it should be noted again that we employed a standard off-the-shelf S_N code which had not been modified for this rather unusual application of ONETRAN. Nevertheless, the computer time comparison given in Table 1 may be taken as an indication that such S_N methods may prove to be advantageous not only conceptually by offering an adjoint capability, but also in computational efficiency.

It should be clear from the generality with which the adjoint method was derived in section III, that its applications are not at all limited to solar radiation transfer problems or any other limited type of problem*. For example, another typical application to the transfer of terrestrial infrared radiation through the atmosphere is quite straightforward. The thermal radiation emitted at groundlevel may be considered as the external radiation source, described by Planck's law and with a spatial delta function in altitude z, $\delta(z)$. If the loss of thermal radiation into space is of interest, then a response function describing the outward directed leakage flux at the top of the atmosphere (altitude $z = \tau$) must be used as an adjoint source term R_{IR} for the adjoint transfer equation; this response function has the form

$$R_{IR}\,(z,\mu,\phi) = \mu\cdot\delta(z-\tau)J(\mu) \quad . \tag{13}$$

Solution of the adjoint transfer equation, Eq. (8), with R from Eq. (13), gives an importance function $I^{+}_{IR}(z,\mu,\phi)$ which quantifies all contributions to the infrared leakage flux from both, external (terrestrial) as well as

*Note added in proof: The adjoint method has recently been applied by Carter, Hovak and Sandford[19] to solve the equation of radiative transfer for polarized light using a Monte Carlo solution technique.

internal (atmospheric) radiation sources. Of course, if atmospheric emissions of infrared radiation are to be considered, then the adjoint Boltzmann operator L^{+} of Eq. (7) has to be slightly modified to include such internal sources.

IV. Conclusions

Our analysis demonstrates in principle and in practice that the computational techniques developed in nuclear technology to solve reactor physics and radiation shielding problems can be applied directly to the solution of solar and infrared radiation transfer problems in the atmosphere. Specifically the highly developed discrete-ordinates (S_N) method is applied to calculate the transmission of solar radiation through clear and polluted atmospheres. The LASL S_N code ONETRAN is shown to solve a typical transmission problem about six times faster than a comparable high-resolution calculation which employs a successive-scattering iterative procedure. More importantly, however, it is also demonstrated how the adjoint method can be used to solve atmospheric radiation transfer problems. Substantial additional computational advantages are derived using the adjoint method in certain cases; an additional factor of 40 in computational efficiency is obtained in our sample case. Moreover, since the adjoint solution to the transfer equation is the basis for many advanced computational methods involving the radiation transfer equation[17,18], the demonstration of its applicability opens many avenues to further improve existing computational capabilities to solve radiation problems in climatology and meterology.

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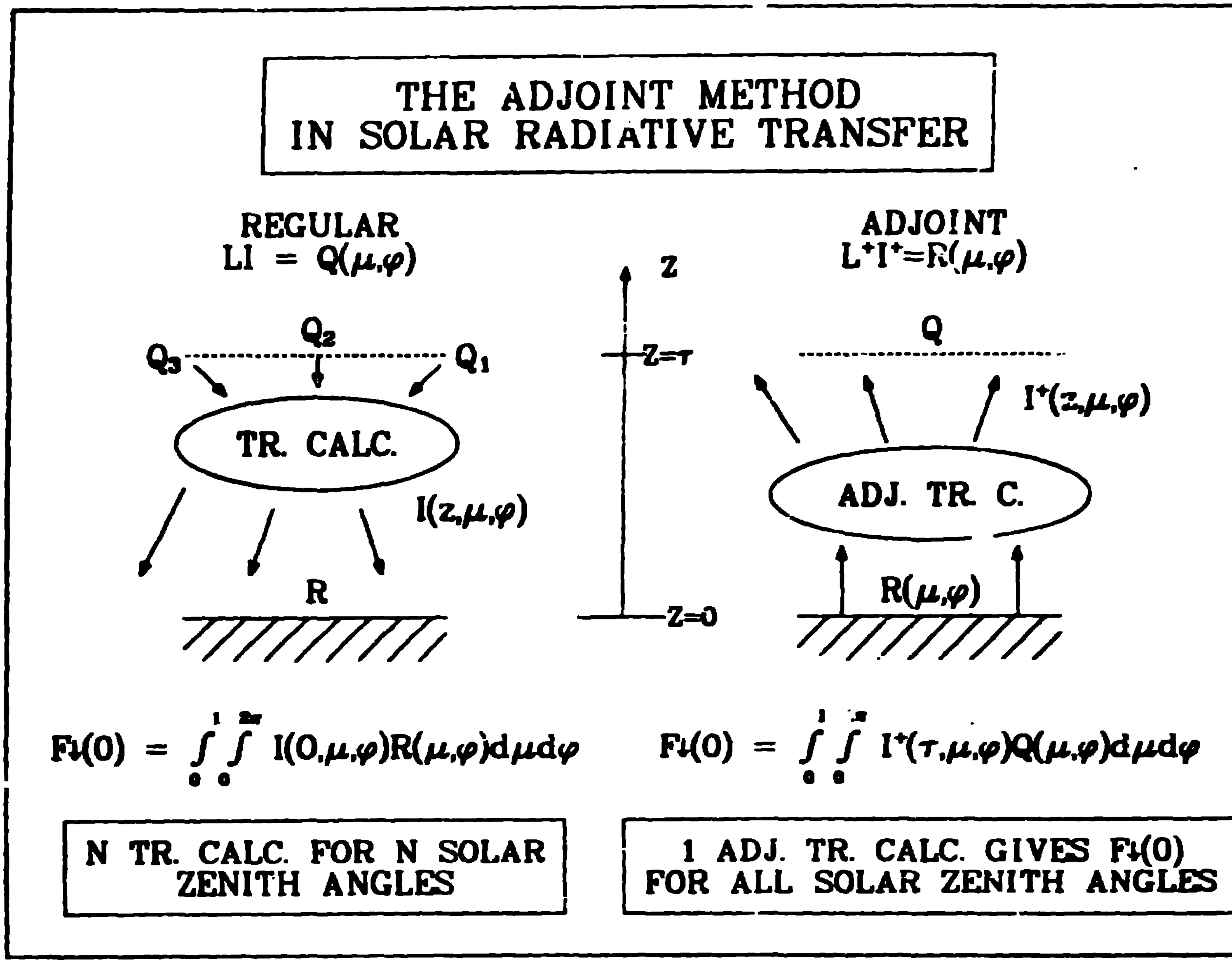

Fig. 1. The concept of the adjoint method compared to the regular method in solar radiative transfer through the atmosphere.

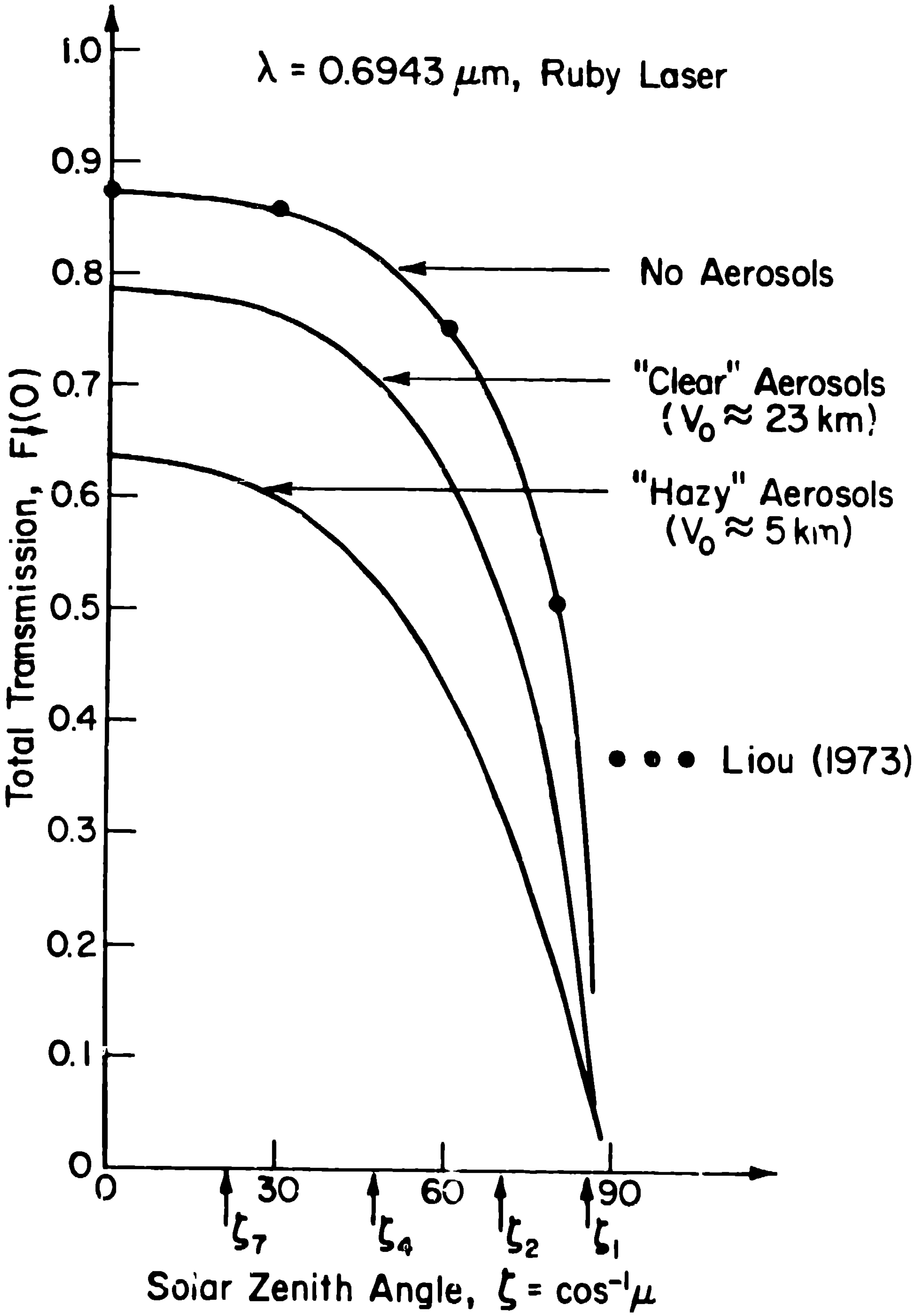

Fig. 2. The diurnal variation of solar irradiance.

COMPUTER TIME COMPARISON

	METHOD	NUMBER OF DISCRETE DIRECT.	CONVERGENCE CRITERION	CPU-TIME ON CDC-7600	
REG. TR. CALC. FOR 1 SOLAR ZENITH ANGLE	SUCCESSIVE SCAT. ITERATIONS (LUTHER, LLL 1974)	91	0.2 %	14.6 SEC.	
	DISCRETE ORD. S_N (GERSTL, LASL 1979)	80	0.2 % (10^{-1} %)	2.4 SEC. (3.1 SEC.)	x6
ADJ. TC. FOR 40 SOLAR Z. ANGLES	ADJOINT DISCR. ORD. S_N (GERSTL, LASL 1979)	80	0.2 %	2.3 SEC	x6x40

Comparison of computer times for the solution of the sample problem by different methods.