Journal of Quantitative Spectroscopy & Radiative Transfer 113 (2012) 721–738

Contents lists available at SciVerse ScienceDirect

Journal of Quantitative Spectroscopy & Radiative Transfer

journal homepage: www.elsevier.com/locate/jqsrt

The NIMO Monte Carlo model for box-air-mass factor and radiance calculations

Timothy D. Hay [a,b,*], Greg E. Bodeker [a,1], Karin Kreher [a], Robyn Schofield [c,2], J. Ben Liley [a], Martin Scherer [a,3], Adrian J. McDonald [b]

[a] *National Institute of Water and Atmospheric Research (NIWA), Lauder, New Zealand*
[b] *University of Canterbury, Christchurch, New Zealand*
[c] *Alfred-Wegener Institute, Potsdam, Germany*

ARTICLE INFO

Article history:
Received 17 August 2011
Received in revised form
11 January 2012
Accepted 4 February 2012
Available online 11 February 2012

Keywords:
Radiative transfer model
Monte Carlo
MAX-DOAS
Box-air-mass factor
Optimal estimation

ABSTRACT

A new fully spherical multiple scattering Monte Carlo radiative transfer model named NIMO (NIWA Monte Carlo model) is presented. The ray tracing algorithm is described in detail along with the treatment of scattering and absorption, and the simulation of backward adjoint trajectories. The primary application of NIMO is the calculation of box-air-mass factors (box-AMFs), which are used to convert slant column densities (SCDs) of trace gases, derived from UV–visible multiple axis Differential Optical Absorption Spectroscopy (MAX-DOAS) measurements, into vertical column densities (VCDs). Box-AMFs are also employed as weighting functions for optimal estimation retrievals of vertical trace gas profiles from SCDs. Monte Carlo models are well suited to AMF calculations at high solar zenith angles (SZA) and at low viewing elevation angles where multiple scattering is important. Additionally, the object-oriented structure of NIMO makes it easily extensible to new applications by plugging in objects for new absorbing or scattering species. Box-AMFs and radiances, calculated for various wavelengths, SZAs, viewing elevation and azimuth angles and aerosol scenarios, are compared with results from nine other models using a set of exercises from a recent radiative transfer model intercomparison. NIMO results for these simulations are well within the range of variability of the other models.

1. Introduction

Solving problems associated with the propagation of light through a spherical, refracting atmosphere, where scattering and absorption may vary with location, is best achieved by applying a Monte Carlo radiative transfer model (RTM). Such models simulate the paths of an ensemble of photons through the atmosphere and estimate the resultant radiation field from the ensemble photon statistics.

An important application for Monte Carlo RTMs is the calculation of air-mass factors (AMFs) for the interpretation of UV–visible Differential Optical Absorption Spectroscopy (DOAS) observations [1,2]. AMFs represent the ratio of the effective optical path through the atmosphere to the vertical path [3,4]. Integrated concentrations of absorbing gases along all light paths contributing to the measured spectra, known as slant column densities (SCDs), are the direct product of the DOAS analysis. SCDs can be converted into vertical column densities (VCDs) through division by AMFs. VCDs are independent of the measurement geometry

* Corresponding author. Now at Laboratory of Atmospheric and Climate Sciences (CIAC), Toledo, Spain. Tel.: +34 659846760.
E-mail address: timothy.hay@ciac.jccm-csic.es (T.D. Hay).
[1] Now at Bodeker Scientific, Alexandra, New Zealand.
[2] Now at School of Earth Sciences, University of Melbourne, Australia.
[3] Now at Department of Environmental Earth System Science, Stanford University, Stanford, USA.

0022-4073/$ - see front matter
doi:10.1016/j.jqsrt.2012.02.005

and light paths, and are therefore more suitable than SCDs for universal interpretation and comparison with other independent measurements.

The box-AMF for a prescribed altitude layer in the atmosphere describes the sensitivity of a SCD measurement, with a given measurement geometry, to the amount of the target trace gas in that layer. Monte Carlo radiative transfer models are well suited to AMF calculations when the optical depth is relatively high, such as in clouds or at high solar zenith angles (SZA) and low telescope viewing elevation angles, because multiple scattering becomes important. Most analytical or deterministic models do not treat multiple scattering well, especially for a three-dimensional inhomogeneous atmosphere. Several important radical species undergo rapid conversion to and from their reservoir species, and their concentrations depend on photolysis rates and therefore on SZA. For these species, whose concentrations vary with SZA along the light path, Monte Carlo models can easily incorporate the effects of this photochemical enhancement. Other applications for Monte Carlo RTMs include analysis of the interaction of solar radiation with three-dimensional clouds in the Earth's atmosphere [5,6], calculation of polarization and radiance at various levels in the atmosphere and ocean [7,8] and simulation of solar radiation during a total eclipse [9].

NIMO was specifically developed for use in the retrieval of trace gas profiles and VCDs from SCDs measured by MAX-DOAS instruments. The model interfaces with a profile retrieval algorithm so the inversion analysis can be fully automated for an entire data set. As a fully spherical model it is well suited for simulations at low elevation viewing angles and high SZA where sphericity significantly influences the photon path lengths through different atmospheric layers.

This paper begins with a brief introduction to the radiative transfer equation (RTE) and the Monte Carlo technique in Section 2, followed by a detailed description of the direct backwards Monte Carlo ray tracing algorithm in Section 3. The calculation of radiances for any solar geometry using the simulation of adjoint photon trajectories in combination with the direct backwards Monte Carlo trajectories is described in Section 4. The calculation of box-AMFs using these photon radiances and trajectories is then described in Section 5. A summary of box-AMF and radiance results from a series of RTM comparison exercises [10] is presented in Section 6, along with some physical interpretation and discussion. NIMO results for these simulations show good agreement within the range of variability of the nine other RTMs that participated in the comparison exercises. These exercises provide an excellent and invaluable tool for testing a new RTM during its development.

2. The Monte Carlo method for solution of the radiative transfer equation

The general integro-differential RTE for unpolarized monochromatic light describes the way the radiance, $I(\mathbf{A},\omega)$, of a light beam changes due to scattering, absorption and emission of photons [11–15], where radiance (or monochromatic intensity) is the radiant power per area per solid angle per wavelength interval:

$$\omega \cdot \nabla I(\mathbf{A},\omega) = -\beta(\lambda,\mathbf{A}) I(\mathbf{A},\omega) + \frac{\beta_s(\lambda,\mathbf{A})}{4\pi} \times \int_{4\pi} I(\mathbf{A},\omega') P(\mathbf{A},\omega\cdot\omega')\, d\omega' + S(\mathbf{A},\omega) \tag{1}$$

The gradient operator, ∇, indicates that the RTE is stated in terms of the rate of change in radiance along the beam in the direction ω. The first term on the right-hand side describes the attenuation in radiance in the direction ω at location $\mathbf{A}$ due to extinction, $\beta = \beta_s + \beta_a$ (see Sections 3.5 and 3.11). The second term describes the increase in radiance at $\mathbf{A}$ due to multiple scattering of photons into the direction ω from direction ω', where $P(\mathbf{A},\omega\cdot\omega')$ is the scattering phase function (see Section 3.8), which is integrated over all directions ω' and normalized by the denominator 4π. The last term is the source function for photon thermal emission, which is negligible in the UV/vis/NIR wavelength region.

The RTE cannot be solved analytically, for anything but the simplest situations, and therefore various numerical methods are applied. RTMs fall into two main classes based on the numerical methods they use to solve the RTE. Firstly, there are deterministic or explicit numerical methods, such as the Discrete Ordinates method [11,14,16–20] and the Spherical Harmonics Discrete Ordinates method [21], which discretise the whole radiation field and iteratively adjust elements of the field until the solution agrees with the RTE. The second class of RTMs is the Monte Carlo methods [7,12,22–30,9], which estimate the desired radiative quantities statistically, with a confidence level dependent on the number of simulated photon trajectories. Monte Carlo methods have the advantage of being able to model specific atmospheric conditions more precisely than deterministic models, but they are usually slower.

Monte Carlo methods [31] use repeated random sampling of a probabilistic model to simulate physical or mathematical processes and they tend to be used where deterministic algorithms are unfeasible or inaccurate. Light propagation in the atmosphere can be regarded as a Markov chain of photon collisions with the medium, in which the probability of each resultant absorption or scattering event is independent of the previous or subsequent events. The Monte Carlo method uses random numbers, uniformly distributed between zero and unity, to simulate events with a probabilistic outcome, such as the scattering angle. The fate of each photon after each collision, whose outcome is prescribed by a probability density function (PDF), is simulated as a random process, much like the spin of a roulette wheel or the roll of dice. However, the outcome of such an event is not selected with uniform likelihood, but in such a way that accumulation of an ensemble of outcomes reproduces the original prescribed PDF.

3. The ray tracing algorithm

NIMO is written in object-oriented Delphi and the model physical environment is defined by a set of objects that represent the atmospheric constituents which absorb or scatter photons (including Rayleigh scattering, aerosols and absorbing trace gases such as O_3 and NO_2). Additional objects