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Radiative transfer modeling through terrestrial atmosphere and ocean accounting for inelastic processes: Software package SCIATRAN

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ABSTRACT

SCIATRAN is a comprehensive software package which is designed to model radiative transfer processes in the terrestrial atmosphere and ocean in the spectral range from the ultraviolet to the thermal infrared (0.18–40 μm). It accounts for multiple scattering processes, polarization, thermal emission and ocean–atmosphere coupling. The main goal of this paper is to present a recently developed version of SCIATRAN which takes into account accurately inelastic radiative processes in both the atmosphere and the ocean. In the scalar version of the coupled ocean–atmosphere radiative transfer solver presented by Rozanov et al. [61] we have implemented the simulation of the rotational Raman scattering, vibrational Raman scattering, chlorophyll and colored dissolved organic matter fluorescence.

In this paper we discuss and explain the numerical methods used in SCIATRAN to solve the scalar radiative transfer equation including trans-spectral processes, and demonstrate how some selected radiative transfer problems are solved using the SCIATRAN package. In addition we present selected comparisons of SCIATRAN simulations with those published benchmark results, independent radiative transfer models, and various measurements from satellite, ground-based, and ship-borne instruments.

The extended SCIATRAN software package along with a detailed User's Guide is made available for scientists and students, who are undertaking their own research typically at universities, via the web page of the Institute of Environmental Physics (IUP), University of Bremen: http://www.iup.physik.uni-bremen.de.

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1. Introduction

The importance of inelastic radiative processes in the atmosphere and ocean has been addressed by many authors [22,38,45,53,73,75,77]. The most important of these processes are the rotational Raman scattering (RRS), vibrational Raman scattering (VRS) and fluorescence by chlorophyll *a* (chl-*a*) and colored dissolved organic matter (CDOM).

In contrast to elastic scattering processes where the incident photons, after interaction with matter (gas, liquid, and solid), preserve the energy, in inelastic processes the frequency of a photon after interaction is shifted to red or blue. A red shift can be observed when part of the energy of the photon is transferred to the interacting matter. This process is referred to as the Stokes Raman scattering. The blue shift occurs when internal energy of the matter is transferred to the photon. This process is known as anti-Stokes Raman scattering [44]. If the energy change of the scattered photon is caused by a change of rotational or vibrational states of molecules, the Raman scattering process is referred to as the rotational (RRS) or vibrational Raman scattering (VRS), respectively. The rotational Raman scattering is important in air but not present in the water, whereas the vibrational Raman scattering is significant in water but of less importance in the air.

The rotational Raman scattering in the atmosphere results predominantly from photons being inelastically scattered by nitrogen and oxygen molecules. The contribution from water vapor and the atmospheric trace gases is in comparison to that of molecular oxygen and nitrogen negligibly small. The width of Stokes and anti-Stokes bands, which comprise numerous narrow rotational lines, is ~1.2 nm at the wavelength of 400 nm. Owing to the red and blue shift, RRS distributes the intensity of the scattered photons over several nanometer. The loss of intensity is proportional to the local intensity of the radiation field whereas the gain is proportional to the intensity at neighboring wavelengths. This leads for example to a filling-in of Fraunhofer lines which was independently discovered by Shefov [66] and Grainger and Ring [26] and is known as the Ring effect.

The VRS phenomenon results from the thermal vibrational properties of the water allowing the energy to be transferred to a specific vibrational mode of the OH bond. For a given pair of energy levels, the energy difference is expressed in terms of a constant frequency shift, e.g., ~3400 cm^{-1} for the OH stretch vibrational mode in water [2]. For example, an incident wavelength of ~400 nm results in the inelastically scattered light in the Stokes band having a wavelength of about 460 nm, i.e., the VRS produces a wavelength shift of about 60 nm in the visible spectral range. The width of the Stokes band in this case is ~8 nm [89,37]. It is much larger than the wavelength shift due to RRS on N_2 and O_2 molecules in the air and also much larger than the width of any Fraunhofer line. In comparison to the Stokes VRS band, the anti-Stokes band is usually much less intense at the ambient temperatures of the world's ocean because it is associated with the relaxation of exited vibrational states, which are not significantly populated at atmospheric and oceanic temperatures [73].

Another well known inelastic process in the ocean is the fluorescence of chl-*a* and CDOM. Fluorescence arises, when an absorbed photon excites an electron of a molecule which then can be transferred to a lower quantum state by undergoing interaction within the molecule or collision processes with other molecules. Thereafter the electron relaxes back to its original state and the emitted photon has lower energy than the original one. In contrast to the RRS and VRS effects, fluorescence occurs only at a lower quantum energy and longer wavelength than the originally absorbed photon. The spectral width of the fluorescence emission bands is in the range 25–100 nm depending on the fluorescence molecule [28,30,71,79].

Inelastic radiative processes such as RRS, VRS, or fluorescence redistribute photons over wavelengths. This results in a filling in of solar Fraunhofer lines, as well as of trace gas absorption structures. This changes the spectral distribution of scattered light in the atmosphere and ocean. Photon redistribution caused by RRS affects atmospheric trace gas retrievals from measurements of scattered light with space-borne instrumentation significantly [80,85,58]. Furthermore, measurements of the filling-in of Fraunhofer lines may be used to estimate cloud top pressure from satellite measurements [33,16] and aerosol properties from both surface and satellite observations [87,88].

The impact of VRS on back-scattered light is similar to that of RRS. Vountas et al. [84] studied the impact of VRS on trace gas retrievals from the GOME satellite instrument and found that neglecting VRS results in significant errors in the DOAS (Differential Optical Absorption Spectroscopy) analysis, e.g., more than 30% for BrO slant columns over clear ocean scenarios. Grossmann et al. [27] included a VRS spectrum to improve their MAX-DOAS (Multi-AXis Differential Optical Absorption Spectroscopy) fit of IO in the marine boundary layer over the ocean especially close to the horizon. A comprehensive study of VRS impacting the NO_2 retrieval was performed by Peters et al. [54].

The VRS spectral features provide useful information about energy transport in the atmosphere and ocean. As recently demonstrated by Dinter et al. [17] the VRS signal retrieved from hyperspectral satellite data can be used as a proxy for the light availability (scalar irradiance) in the global ocean, which is an important parameter for both estimating phytoplankton primary production from satellite data and assessing the heat content in the surface ocean.

In the UV spectral range, the filling-in of Fraunhofer lines by VRS in the ocean is decreased with increasing phytoplankton and CDOM concentration as they both absorb UV radiation. This characteristic was used to retrieve the oceanic chlorophyll content by Joiner et al. [35].

The information content of the filling-in signal originating from CDOM and chl-*a* fluorescence was studied among others by Wolanin et al. [91,90]. In particular, it was demonstrated that the information from chlorophyll fluorescence measurements can be used to assess the physiological state of phytoplankton to further improve the knowledge of biogeochemical cycles, productivity and physiology of marine environments [4,18], whereas the CDOM-fluorescence signal