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Numerical determination of visible/NIR optical constants from laboratory spectra of HED meteorites

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ABSTRACT

Radiative transfer models in particulate media (Hapke, 1981, 1993, 2012b; Shkuratov et al., 1999) are the most versatile tool that can be used to retrieve both composition and surface physical properties from observation of asteroids and other atmosphereless bodies of the Solar System. One caveat is that these methods require as input a sufficiently comprehensive set of optical constants of suitable template materials. These optical constants are the real and imaginary parts of the refractive indexes of the material as function of wavelength, and have to be derived from laboratory measurements of samples of minerals and meteorites. Optical constants can be calculated from a variety of types of measurements, and each has its problems and limitations. In particular, a problem with the determination of optical constants from measurement of reflectance is that the measurements need to be themselves interpreted using radiative transfer models. This is an issue because the number of parameters used in the most accurate versions of the radiative transfer models is large, and for most of the samples many of these parameters were not measured independently. As a result, attempts in the literature to retrieve optical constants from reflectance measurements tend to assume values for the unknown parameters, which can lead to uncertainties in the retrieved optical constants that can be difficult to quantify. In this work we propose a numerical method that allows the simultaneous inversion of the optical constant and the model parameters. This model is then applied to a set of reflectance spectra of 5 HED meteorites from the RELAB database that were measured with the same setup for samples with several particle size intervals. Our results indicate that our method is able to retrieve optical constants which are able to reproduce the measured reflectance of the samples over a large range (25–500 μm) of particle diameters. It is also found that the solutions obtained in this way are non-unique, in the sense that many combination of the model parameters can yield different sets of optical constants that fit equally well the reflectance spectra. Thus, in the absence of the independent determination of at least some of the model parameter the method is unable to decide which solution correspond to the physical optical constants of the materials. Even so, the dispersion of the model parameters (in particular effective particle diameter and porosity) for acceptable solutions (defined as the ones that reproduce the measured reflectance spectra at all size range with residues smaller than 10%) is within a radius of around 30% of the value of the best fit solution for each parameter. Given the ability of the optical constants derived with this method to reproduce the sample spectra over a large range of particle sizes, they can be used without other restriction to assess if a given meteorite assemblage is contributing to the observed spectra of asteroids. However, quantitative informations that can also be derived using these optical constants, like particle sizes, porosity and volumetric fractions of each end-member in a mixture should be regarded only as rough estimates.

1. Introduction

The remote determination of the composition of Solar System bodies depends on the existence of laboratory measurements of the spectra of minerals and meteorites. These spectra can be then used to constrain the composition of those bodies in several different ways, each with its own advantages and pitfalls: direct comparison, spectral parameterization/modelization, and radiative transfer models (Gaffey et al., 2002; Reddy et al., 2015).

The first method, direct comparison (which is also referred in the literature as curve matching) is the easiest to use. This method

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is useful to assess similarities and suggest possible analogs. Problems with this approach are that the shape of the spectrum also depend on the texture of the sample and on the geometry of the measurements, and that the spectra of airless bodies can be affected by space weathering effects (Gaffey et al., 2002).

The second method, the parameterization of spectra of mineral end-members, is made through the quantification of spectral characteristics that can be used as diagnostic of composition and is most useful for spectra dominated by olivine/pyroxene bands. Parameters and calibrations derived in this way are, to some extent, unaffected by geometry, texture, or space weathering (Cloutis and Gaffey, 1991; Gaffey et al., 2002; Reddy et al., 2015; Ruesch et al., 2015). The application of the method is straightforward if the observed spectra has sufficient overlap to the spectra used to derive the calibrations. This method however is of limited, if any, use for assemblages whose spectra is not characterized by the presence of absorption bands, and is incapable of estimating the contribution of components with featureless spectrum. To address the issue of mixtures of end-members it is necessary to measure the spectra of a suitable amount of carefully prepared samples that span the range of possible mixing fractions. Similarly, constraints and calibrations derived from laboratory measurement of mineral end-members are needed in order to apply the Modified Gaussian Model (Clenet et al., 2013; Sunshine and Pieters, 1993) to the spectra of Solar System objects, which attempts to model absorption bands in reflectance spectra as the sum of Gaussian features plus a continuum that is linear in energy. Here laboratory spectra are used to constrain the parameters of the Gaussians used to describe the bands of each end-member. This method can in principle handle mixtures of an arbitrary number of end-members without the need of dedicated measurements of laboratory-prepared mixed samples, but in practice the uniqueness of the solutions derived is not guaranteed. The method is also of limited use for materials whose spectrum is not dominated by absorption bands, and also cannot constrain the presence of featureless components in the spectra.

In all those methods the measured spectra are used directly, which means that constraints obtained refer explicitly, to some degree, to the geometry and the texture (whether the sample was a slab or particulate, grain size ranges, etc) of each measurement. That is not the case of radiative transfer models in soils (the most used variety of which being the Hapke models) which can in principle handle mixtures of an arbitrary number of end-members, provide constraints to the presence of spectrally neutral mineral phases, and simulate almost any observational geometry and surface textures, as well as model the effects of space weathering (Hapke et al., 2009; Pieters et al., 2000). This type of method can also be used to assess the composition of bodies with surfaces dominated by materials whose spectrum does not present conspicuous spectral absorptions, as well as to constrain the presence of such materials in mixtures. One caveat with this kind of methods is that in order to obtain an unique solution for a set of presumed end-members it in general requires, besides a spectrum, additional information about the object like geometric albedo or measurements at different observational geometries, since the number of parameter and their functional dependence in the models can result in non-unique solutions (Baratoux et al., 2006; Cord et al., 2003; Helfenstein and Shepard, 2011; Schmidt and Fernando, 2015; Shepard and Helfenstein, 2011).

Other major issue here is that these methods need as input the spectra of the optical constants of the end-members, which have in turn to be derived from their reflectance or transmittance spectra. This is a problem since the determination of optical constants from reflectance spectra is not straightforward and presents several difficulties. One first decision to be made here is on what radiative transfer model to use, with Shkuratov (Shkuratov et al., 2005) and Hapke models being the ones most commonly used in the literature. Hapke models in particular have been evolving over the years to incorporate effects like opposition surge, macroscopic roughness and porosity of the particulate sample. For Hapke models it is also necessary to choose a model to calculate the single scatter albedo from the optical constants. The measured spectrum depends therefore on several parameters concerning the texture of the sample and the geometry of the measurement. Ideally, the number of free parameters can be reduced by an adequate choice of the measurement geometry, and by a careful determination of the particle size distribution and the porosity of the sample. An independent determination of the real part of the optical constants in at least one wavelength is also necessary in order to derive optical constants in the visible to NIR range.

At this point there is a large number of reflectance spectra of minerals and meteorites in public databases (i.e. Pieters, 1983; Clark et al., 2003; Milliken et al., 2016). Many of those spectra were obtained from particulate samples that were separated into diameter ranges through sieving, and the only available information about the diameter distribution of the particles is the minimum and maximum particle sizes that are expected to be in the sample, given by limiting diameters of the sieve's holes used in the sample preparation. Usually there is no direct estimation of the porosity of the sample, and for most materials there is also no direct measurement of the real part of the optical constants in the visible or near infrared.

In this work we investigate the problem of retrieving the optical constants from reflectance spectra of particulate samples with unknown porosity or real refractive index, and for which the information of the size distribution is limited to the assumed maximum and minimum diameters set during the sample preparation. The objective is to develop a method that uses spectra of the same material measured from sample with different particle diameter limits in order to obtain the spectrum of the imaginary part of the refractive index of the materials, its real part and also the effective diameters and porosities of each sample. This is done by using a genetic algorithm to simultaneously invert the spectra of each sample to obtain the corresponding spectra of the imaginary refractive index k_λ, while requiring that the difference among k_λ for all sample is minimized. We are particularly interested in the possibility of retrieving useful optical constants from meteorite spectra. Meteorites are ready-made assemblages of materials that are representative of the composition of at least part of the asteroids, and the use of meteorite optical constants in radiative transfer methods would provide a powerful tool to establish or strengthen the links between meteorites and asteroids. Concerning radiative transfer models, a difference between using minerals or meteorites as end-members is that mineral particles in principle are homogeneous, whereas meteorite particles are be themselves composed by mixtures of different mineral particles with smaller sizes and in close proximity. In this sense, optical constants of meteorites could be regarded as the effective average optical constants of these mixed assemblages. Therefore, as long as these effective optical constants do not vary with particle size, their use in radiative transfer models would in principle be subjected to the same limitations as pure mineral end-members. With this in sight, the method presented here is then applied to a set of spectra of five HED meteorites in order to verify whether an unique, physically realistic solution can be obtained in this way and, if not, how useful the solutions obtained can still be to the problem of constraining the composition of Solar System bodies. In Section 2 we discuss the reflectance model adopted and its hypothesis; In Section 3 we present a sample of 5 meteorites, each with spectra of sample separates within several diameter ranges, that will be used to test the inversion methods and perform an initial inversion test. A thorough exploration of parameter space is performed in Section 4 in

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