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Solar spectral performance of nanopigments

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ABSTRACT

Solar spectral behavior of nanopigments has been an important issue in many practical relevance due to their tunable properties. There are extensive literatures on radiative transfer through pigmented coating but they are generally restricted to a small range of materials with specific properties and particular applications. Current study, on the other hand, concerns with a comprehensive look at contribution of fundamental characteristics of nanopigments on spectral behavior of the pigmented coatings. In order to accomplish this goal, a Discrete Ordinate Method (DOM), known as Multi Flux (MF) model in color science, has been applied on spherical particles embedded in nonabsorbing medium, and their optical responses including reflectance, transmittance and absorption has been studied over solar spectrum, with special emphasis on VIS region. The effect of various indices of refraction, particle sizes and volume fractions has been further investigated. Obtained results reveal that, pigments with different fundamental and morphological structures represent interesting optical behavior which is very promising in optimization of spectrally selective pigmented coatings. The results from MF model were subsequently validated using spectrophotometric measurements on Titanium dioxide nanopigments coated on white polyester substrate, which represented a good agreement with collected data from MF model.

1. Introduction

Pigmented coatings are semitransparent media which can reflect, transmit and absorb the incident radiation. Thanks to optical properties of nanopigment particles, they have been provided several unique functions in many engineering applications such as energy [1,2], environment [3,4] and textile industry [5,6].

To start, Ultraviolet irradiation in solar spectrum, which covers (250–400) nm, has the potential to cause many negative effects on the body as well as industrial products such as polymers and paints. Therefore, it is recommended to protect such surfaces from the UV radiation. Using UV absorbing nanopigments, such as Titanium dioxide nanopigments, is an appropriate way to efficiently protect surfaces from UV attack [7]. Besides, in Visible part of electromagnetic spectrum, (400–700)nm, nanopigment particles can provide whiteness, brightness and opacity to products such as paints, plastics, papers, inks and synthetic fibers [8]. Absorption of solar irradiation in NIR region can potentially raise temperature inside cars and buildings [9,10]. The similar effect can also be observed in clothing and textiles [11]. “Cool pigments” or “NIR reflecting pigments” have been the subject of many studies, which are involved in designing temperature moderating coatings [12]. According to mentioned remarks, designation and simulation of a coating with predetermined optical properties has been an important issue and subject of many scientific researches [13].

Different approaches have been developed for modeling of radiative behavior of semi-transparent particles in multiple scattering regimes [14,15], among them, a quite practical method is based on the solution of the Radiative Transfer Equation (RTE), due to its conceptual simplicity. One of the most commonly used methods for solving radiative transfer equation is Discrete Ordinate Method (DOM), which was first introduced with Chandrasekhar in 1940 [16]. In the DOM, the continuous 4π solid angle range around the scattering media is divided into a finite number (n) of discrete directions or ordinates. Afterwards, the RTE could be solved as an ordinary algebraic equation with appropriate weighting along each direction, and numerical quadrature replaces the integral over direction in the scattering term [17–19].

One of the earliest methods of dealing with DOM equation is to consider two angular components of forward and the reverse directions with appropriate corrections for surface reflection. This one dimensional radiation transfer theory is known as two-flux approximation or Kubelka-Munk (KM) theory, which assumes diffused light only. Kubelka-Munk theory has been used extensively in color science and technology in order to study reflectance and transmittance of materials [20–22]. The four-flux model of Maheu, Letoulouzan and Gouesbet (MLG), on the other hand, is the extension of two-flux approximation,

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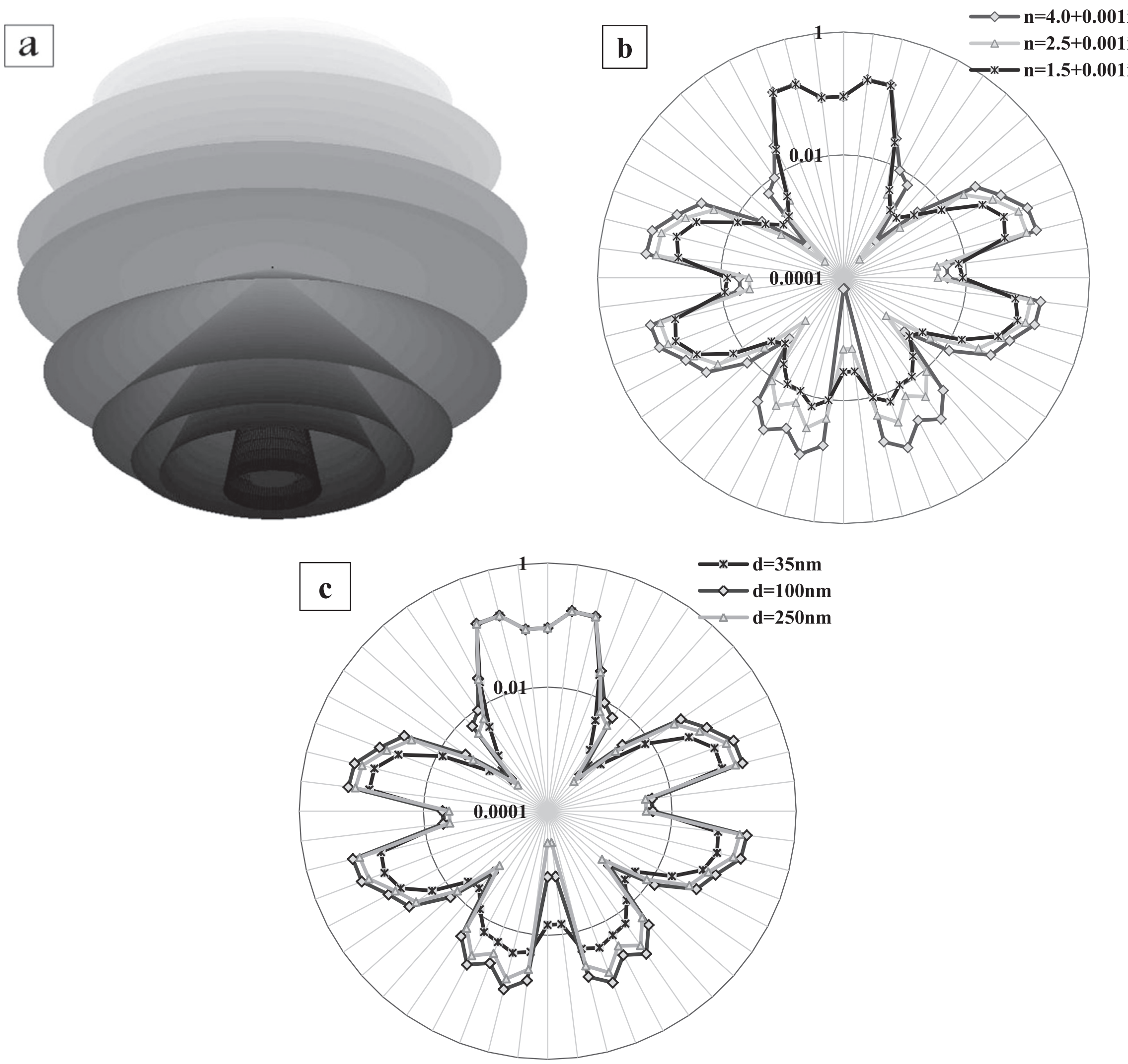

Fig. 1. (a) Space discretization for multi-flux model, and angular distribution of scattered light for a pigmented layer with the thickness of 1.5 μm and f_v=5.0% for (a) particles with different complex refractive index (for d=100 nm) and (b) diameters (for n=4.0+0.001i), at λ=420 nm.

which considers two collimated and diffuse light beams propagating in the forward direction and two collimated and diffuse beams propagating in the backward direction [23–25].

The more accurate and general case, Multi-Flux or N-flux model, considers N flux channels, in which, the number of flux channels can exceed 250 and the light path could be diffuse or collimated and in forward or backward directions. Multi-flux theory provides a procedure to figure out the reflectance and transmittance of a particulate system from its fundamental characteristics such as particle size and refractive index [26–29].

According to extent and importance of optical applications of nanopigment particles, present paper aims to theoretically predict the spectral behavior of mono-dispersed nanopigments, with different refractive indices, sizes and volume fraction, embedded in non-absorbing resin with n=1.54, in Ultra Violet (UV), Visible (VIS) and Near Infrared (NIR) regions of electromagnetic spectrum, and to show how this properties can alter optical behavior of a pigmented layer. In order to model radiative transfer through the pigmented layer, discrete ordinate method, namely Multi Flux model, has been conducted on obtained database from Mie theory. The effect of complex index of refraction, particle size and concentration of nanopigments on spectral behavior of the layer has been investigated.

At the next place, Titanium dioxide (TiO_2) nanopigments have been selected to validate the predicted results. To do this, spectral reflectance, absorption and transmittance of TiO_2 particles has been reproduced using MF model. Afterwards, spectrophotometric measurements have been performed on a white polyester substrate, which was coated with TiO_2 nanopigments with various sizes and concentrations. And ultimately, obtained results have been discussed in details.

2. Materials and methods

2.1. Mathematical model

Multi-flux calculations were performed on pigmented layers with regard to Mudgett and Richard's procedure in treatment of RTE for closely packed pigmented media [30,31]. A wide variety of nanopigment particles with various diameters, d=35–250 nm, and index of refraction, N=n_1+ki, in which n_1 and k varies in the range of (1.5–4.0) and (0.001–1.0) respectively, has been investigated. Front surface of the media is assumed to be illuminated by ideal diffuse light, which is in the forward direction inside an angle range of $\pm \pi/2$ and has equal energy over the entire range of these angles. A polar coordinate system of 26 unequal angular segments, which covers different ranges of angles from perpendicular to horizontal,