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Calculation of the reflectance of dense particulate media based on the superposition T-matrix method combined with bidirectional power flux theory

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Optics of particulate media is a very important topic in many areas of research and technology ranging from traditional paints and functional pigments [1] to light generation in random lasers [2]. Bidirectional power flux Kubelka-Munk theory [3] is often used to estimate the reflectance of particulate media by extrapolating data generated with Mie codes towards a bulk response. Consequently the applicability of this method is limited to samples with low particles density, where coherent multiple scattering can be neglected. Here we propose a more accurate approach to simulate reflectance from dense particulate systems and demonstrate our method for a dense composite, filling fraction 25%, of randomly distributed hematite spheres with a diameter of 250nm, which is illuminated under normal incidence.

We start with a T-matrix method [4] based calculation of the directional power flux of light in a cylindrical volume (750nm height and 4μm diameter) containing a randomly distributed ensemble of 287 particles, see Figure 1. The illumination direction is normal to the cylinder's base and the surrounding medium is polymer with a refractive index n =1.5. The scattering coefficients obtained from the superposition T-matrix simulations are used to compute the electric and magnetic fields on the cylinder bases. These field distributions are used to compute the power flux needed to estimate reflectance and transmittance of this thin layer of particles. The whole particulate medium is now approximated by an infinite stack of layers, the reflectance of which is calculated based on the assumption that an additional layer will not alter it (see black diamonds in Figure 2). Strictly speaking the so calculated reflectance describes that of a 4μm wide half-infinite cylinder of particulate medium embedded in polymer. For the more common situation, of an interface between air and a polymer based particulate medium, the obtained reflectance has to be corrected to account for the power flow across the air-polymer interface. The corrected version of the reflectance (Figure 2 blue circles) is in a good agreement with measurements performed in comparable systems (green line in Figure 2). Deviations in the long wavelength range are most likely caused by the ensemble's edge scattering, which might be resolved by increasing the layer's lateral dimensions. The proposed approach can be used to study and optimize light interaction with dense particulate media where coherent multiple scattering effects cannot be disregarded because for example of particle aggregation.

Figure 1. Cluster of N=287 mono-disperse particles occupying a cylinder. Electric and magnetic fields are computed on the planes above and below the cluster.	**Figure 2.** Measured and computed reflectance spectra for 200nm large hematite particles embedded in a polymer matrix.

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