HARRICK Scientific Products
Solutions in Optical Spectroscopy

What is Kubelka-Munk?

Diffuse reflectance was developed to facilitate analysis of materials such as papers and powders in their neat state. The common characteristic of these materials is their internal inhomogeneities. The propagation of light through such inhomogeneous media differs significantly from the propagation of light in a homogeneous material, since the light scatters off points in its path.

Thus the key to the theoretical description of diffuse reflection lies in the description of the propagation of light through inhomogeneous materials. However, only approximate descriptions exist. The most widely used model for diffuse reflection is the one put forward by Kubelka and Munk.

The Kubelka-Munk (K-M) model has a particularly simple solution in the case of semi-infinite samples. All the geometric peculiarities of the inhomogeneous sample are condensed into a single parameter, the scattering coefficient s. The diffuse reflectance R_∞ is given as:

$$R_\infty = 1 + \frac{k}{s} - \sqrt{\frac{k}{s}\left(2 + \frac{k}{s}\right)}$$

where *k* is the absorption coefficient of the sample ($k = 4\pi\,{}^{\kappa}\!/_{\lambda}$); where λ is the wavelength).

This relatively simple form is easily solved for k/s yielding the familiar K-M transform:

$$\frac{k}{s} = \frac{(1 - R_\infty)^2}{2R_\infty}$$

The K-M transform of the measured spectroscopic observable is approximately proportional to the absorption coefficient and hence is approximately proportional to the concentration.

A few words must be said about the scattering coefficient. This coefficient was introduced into the theoretical description of diffuse reflection as a semi-empirical parameter to account for the internal scattering processes. The scattering coefficient s is, in fact, dominated by particle size and refractive index of the sample. It is not a strong function of the wavelength or the absorption coefficient, so the K-M model considers it a constant. In reality, the scattering coefficient does vary slowly with wavelength. More importantly, it changes significantly with packing density, so care should be taken to pack powdered samples as reproducibly as possible if quantitative results are required.

Expression (2) is the analog of the absorbance transformation in transmission spectroscopy. Due to it simplicity, it has been widely incorporated as the diffuse reflectance transform in the standard infrared spectroscopy software of commercial FT-IR spectrometers.