The Kubelka-Munk Theory of Reflectance

This theory was originally developed for paint films but works quite well in many circumstances for paper. It is not, however, terribly good for dyed papers (or very dark, unbleached papers) when light absorption reaches a high level. A limiting assumption is that the particles making up the layer must be much smaller than the total thickness. Both absorbing and scattering media must be uniformly distributed through the sheet. Ideally, illumination should be with diffuse monochromatic light and observation should be of the diffuse reflectance of the paper. The theory works best for optically thick materials where > 50 % of light is reflected and < 20 % is transmitted.

Kubelka and Munk

**Figure 1** Consider light of intensity $I_0$ incident on a non-glossy piece of paper of thickness $X$ and reflectance $R$. Behind this piece of paper is a surface of reflectance $R'$. The light which re-emerges from the top surface of the paper after scattering, absorption or transmission has intensity $I$. At a distance $x$ from the bottom surface of the paper there is a thin lamina of thickness $dx$ and scattered light is incident on it which is travelling both upwards and downwards through it with intensities $i_R$ and $i_T$, respectively.

Define:
K is the Absorption Coefficient ≡ the limiting fraction of absorption of light energy per unit thickness, as thickness becomes very small.

S is the Scattering Coefficient ≡ the limiting fraction of light energy scattered backwards per unit thickness as thickness tends to zero.

The effect of the material in a thin element dx on $i_T$ and $i_R$ is to:
- decrease $i_T$ by $i_T(S + K) dx$ (absorption and scattering)
- decrease $i_R$ by $i_R(S + K) dx$ (absorption and scattering)
- increase $i_T$ by $i_R S dx$ (scattered light from $i_R$ reinforces $i_T$)
- increase $i_R$ by $i_T S dx$ (scattered light from $i_T$ reinforces $i_R$).

So:

\[ -di_T = -(S + K)i_T dx + i_R S dx \] \[ di_R = -(S + K)i_R dx + i_T S dx, \]

where $x$ is measured from the bottom of the sheet, i.e. upwards in figure 1, which affects the signs.

Divide [1] by $i_T$ and [2] by $i_R$ and add together:

\[ \frac{di_R}{i_R} - \frac{di_T}{i_T} = d \left\{ \ln \left( \frac{i_R}{i_T} \right) \right\} = -2(S + K) dx + S \left( \frac{i_T}{i_R} + \frac{i_R}{i_T} \right) dx. \] \[ [3] \]

Define $R = I/I_0$ as reflectance of sheet and $r = i_R/i_T$ as reflectance of increment and:
\[d(\ln r) = \frac{dr}{r}.
\]

So, \(\frac{dr}{r} = \left(-2(S+K) + S\left(\frac{1}{r} + r\right)\right)dx,
\]

and, rearranging:

\[
\int_r^R \frac{dr}{r\left(\frac{1}{r} + r\right) - 2\left(1 + \frac{K}{S}\right)} = S\int_0^x dx
\]

\[
\int_r^R \frac{dr}{1 + r^2 - 2\left(\frac{S+K}{S}\right)r} = S\int_0^x dx, \tag{4}
\]

which gives \(R\) in terms of \(S, K\) and \(R'\).

Let \(a = \frac{S+K}{S} = 1 + \frac{K}{S}\) and equation \(4\) becomes:

\[
\int_r^R \frac{dr}{r^2 - 2ar + 1} = S\int_0^x dx. \tag{5}
\]

The LHS (Left hand Side) integration is achieved by partial fractions:

Put \(r^2 - 2ar + 1 = 0\) and solve,

\[
r = \frac{2a \pm \sqrt{4a^2 - 4}}{2} = a \pm \sqrt{a^2 - 1}
\]

so \(r^2 - 2ar + 1 = \left(r - a - \sqrt{a^2 - 1}\right)\left(r - a + \sqrt{a^2 - 1}\right)
\]

and \(\frac{1}{r^2 - 2ar + 1} = \frac{A}{r - a - \sqrt{a^2 - 1}} + \frac{B}{r - a + \sqrt{a^2 - 1}}\).

Putting the RHS over a common denominator yields:

\[
A\left[r - a + \sqrt{a^2 - 1}\right] + B\left[r - a - \sqrt{a^2 - 1}\right] = 1.
\]

Comparing coefficients of \(r:\)

\[
A + B = 0. \tag{6}
\]
Comparing constants:
\[ A\left(-a + \sqrt{a^2 - 1}\right) + B\left(-a - \sqrt{a^2 - 1}\right) = 1. \]

Using [6], \[ B = \frac{-1}{2\sqrt{a^2 - 1}} \]
\[ A = \frac{1}{2\sqrt{a^2 - 1}}. \]

Equation [5] becomes:
\[ \int_{R'}^R \frac{1}{r - a - \sqrt{a^2 - 1}} - \frac{1}{r - a + \sqrt{a^2 - 1}} \, dr = 2\sqrt{a^2 - 1} \int_0^X dx \]
and,
\[ \ln\left(\frac{r - a - \sqrt{a^2 - 1}}{r - a + \sqrt{a^2 - 1}}\right) \bigg|_{R'}^R = 2\sqrt{a^2 - 1} SX. \]
\[ \ln\left[\frac{R - a - \sqrt{a^2 - 1} \cdot R' - a + \sqrt{a^2 - 1}}{R - a + \sqrt{a^2 - 1} \cdot R' - a - \sqrt{a^2 - 1}}\right] = 2\sqrt{a^2 - 1} SX \]

It is usual to substitute \[ b = \sqrt{a^2 - 1} \]
giving,
\[ \ln\left(\frac{R - a - b \cdot R' - a + b}{R - a + b \cdot R' - a - b}\right) = 2bSX \quad [7] \]

Consider the limiting condition where \( X = \infty \), \( R = R' = \infty \) and \( R' \) can take any value, since no light gets to it, so we can set \( R' = 0 \).
The LHS of [7] must equal \( \infty \), which means that the denominator must equal 0 and:
\[ R_\infty = a - \sqrt{a^2 - 1} \quad [8] \]
\[ = 1 + \frac{K}{S} - \frac{K^2}{S^2} + \frac{2K}{S}. \quad [9] \]

Note that equation [9] can be approximated to
\[ R_\infty = 1 - \sqrt{\frac{2K}{S}}. \]

Equation [9] implies that \( R_\infty \) can only be \( < 1 \) if \( K \) is non-zero. This is reasonable because, if there is no absorption, all light must be scattered until it reappears from the top surface of the paper!
From [8], $a - R_\infty = \sqrt{a^2 - 1}$

square and rearrange: $a = \frac{R_\infty^2 + 1}{2R_\infty}$

$$1 + \frac{K}{S} = \frac{R_\infty^2 + 1}{2R_\infty}$$

$$\frac{K}{S} = \frac{(R_\infty - 1)^2}{2R_\infty}$$

$$\sqrt{a^2 - 1} = \sqrt{\left(\frac{R_\infty^2 + 1}{4R_\infty^2}\right) - 1}$$

$$-\frac{1}{2R_\infty}\sqrt{R_\infty^4 - 2R_\infty^2 + 1}$$

and, by convention, $b = \frac{1 - R_\infty^2}{2R_\infty}$.

Substitute for $a$ and $b$ in equation [7] and simplify:

$$SX = \frac{R_\infty}{1 - R_\infty^2} \ln \left[ \frac{(R' - R_\infty)}{(R' - \frac{1}{R_\infty})(R - R_\infty)} \right]$$

Up to now $X$ is in length units and $K$ and $S$ are in appropriate dimensions to leave $SX$ and $KX$ dimensionless.

Van den Akker (see, for example, Handbook of Paper Science) says we can use an incremental grammage layer $dW$ and redefine:

- $k$ is fractional absorption loss of radiant flux per unit basis weight,
- $s$ is fractional scattering loss of radiant flux per unit basis weight

and replace $KX$ and $SX$ with $kW$ and $sW$ in all solutions and graphical aids.

$k$ is typically $< 2$ m² kg⁻¹ for coated and uncoated fine papers made from bleached chemical pulps, is $3 < k < 6$ m² kg⁻¹ for mechanical pulps and is around $14$ m² kg⁻¹ for unbleached kraft pulps.

$s$ is $> 50$ m² kg⁻¹ for filled and coated fine papers, $20 < s < 40$ m² kg⁻¹ for bleached and unbleached chemical pulps and is typically $40 < s < 70$ m² kg⁻¹ for mechanical pulps.

To differentiate $s$ and $k$ from $S$ and $K$, we often call them "specific scattering coefficient" and "specific absorption coefficient".
It is also useful to make R the subject of equation [11]:

\[
\exp\left(\frac{(1-R^2)SX}{R_\infty}\right) = \frac{(R'-R_\infty) R - \frac{1}{R_\infty}}{(R' - \frac{1}{R_\infty}) (R - R_\infty)}
\]

\[
(R - R_\infty)\exp\left(\frac{(1-R^2)SX}{R_\infty}\right) = \frac{(R'-R_\infty) R - \frac{1}{R_\infty}}{R' - \frac{1}{R_\infty}}.
\]

Re-arranging:

\[
R\exp\left(\frac{(1-R^2)SX}{R_\infty}\right) - \frac{R'-R_\infty}{R' - \frac{1}{R_\infty}} = \frac{-1}{R_\infty} \frac{R'-R_\infty}{R' - \frac{1}{R_\infty}} + R_\infty \exp\left(\frac{(1-R^2)SX}{R_\infty}\right)
\]

\[
\text{So, } R = \frac{\frac{1}{R_\infty} (R'-R_\infty) - R_\infty \left(\frac{R'-1}{R_\infty}\right) \exp\left(\frac{1}{R_\infty} - R_\infty\right) SX}{(R'-R_\infty) - \left(\frac{R'-1}{R_\infty}\right) \exp\left(\frac{1}{R_\infty} - R_\infty\right) SX} \quad [12]
\]

Both equations [11] and [12] are used to determine basis weight corrected opacity.

\[
\text{Opacity} = \frac{R_0}{R_\infty}
\]

R_0 depends on basis weight, so when handsheets, which differ from the standard weight are used, R_0 must be corrected. Obviously, R_\infty does not change.

From equation [11], scattering coefficient s can be calculated by substituting R = R_0 and R’=0:

\[
s - \frac{1}{W} \left(\frac{R_\infty}{1-R^2}\right) \ln\left\{\frac{R_0 - \frac{1}{R_\infty}}{R^2 \frac{R_\infty}{R_0} - R_\infty}\right\} \quad [13]
\]

Now, using equation [12], R_0 for the standard grammage, W_{std} can be calculated:
\[ R_0 = \frac{\exp\left\{ \left( \frac{1}{R_\infty} - R_\infty \right) sW_{\text{nl}} \right\} - 1}{\frac{1}{R_\infty} \exp\left\{ \left( \frac{1}{R_\infty} - R_\infty \right) sW_{\text{nl}} \right\} - R_\infty}. \]