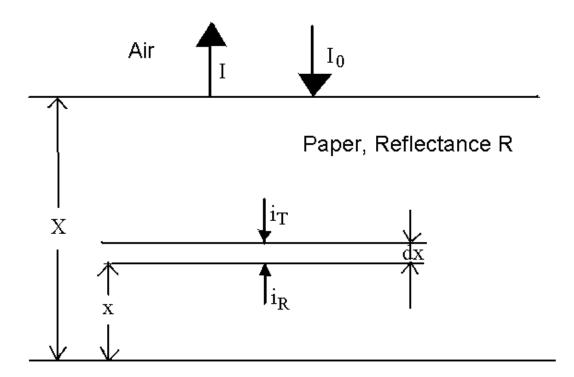
The Kubelka-Munk Theory of Reflectance

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 Zeit. Für Tekn. Physik, <u>12</u>, p593 (1931).



Backing, Reflectance R'

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 \equiv 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:

$$- \operatorname{di}_{T} = -(S + K)i_{T} dx + i_{R} S dx$$

$$\operatorname{di}_{R} = -(S + K)i_{R} dx + i_{T} S dx,$$
[1]

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:

$$\frac{\operatorname{di}_{R}}{i_{R}} - \frac{\operatorname{di}_{T}}{i_{T}} = \operatorname{d}\left\{\ln\left(\frac{i_{R}}{i_{T}}\right)\right\} = -2(S + K)\operatorname{dx} + S\left(\frac{i_{T}}{i_{R}} + \frac{i_{R}}{i_{T}}\right)\operatorname{dx}.$$

$$\left\{
\begin{array}{l}
\operatorname{Note that}: \\
\frac{\operatorname{d}\left[\ln\left(\frac{i_{R}}{i_{T}}\right)\right]}{\operatorname{dx}} = \frac{\operatorname{d}\left[\ln\left(i_{R}\right) - \ln\left(i_{T}\right)\right]}{\operatorname{dx}} \\
= \frac{\partial \ln\left(i_{R}\right)}{\partial i_{R}} \frac{\operatorname{di}_{R}}{\operatorname{dx}} - \frac{\partial \ln\left(i_{T}\right)}{\partial i_{T}} \frac{\operatorname{di}_{T}}{\operatorname{dx}}
\end{array}\right\}$$

$$= \frac{1}{i_{R}} \frac{\operatorname{di}_{R}}{\operatorname{dx}} - \frac{1}{i_{T}} \frac{\operatorname{di}_{T}}{\operatorname{dx}}$$

$$\operatorname{d}\left[\ln\left(\frac{i_{R}}{i_{T}}\right)\right] = \frac{\operatorname{di}_{R}}{i_{R}} - \frac{\operatorname{di}_{T}}{i_{T}}$$

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

and, rearranging:

$$\int_{\mathbb{R}^{l}}^{\mathbb{R}} \frac{dr}{r \left\{ \left(\frac{1}{r} + r \right) - 2 \left(1 + \frac{K}{S} \right) \right\}} = S \int_{0}^{\mathbb{X}} dx$$

$$\int_{\mathbb{R}^{l}}^{\mathbb{R}} \frac{dr}{1 + r^{2} - 2 \left(\frac{S + K}{S} \right) r} = S \int_{0}^{\mathbb{X}} dx,$$
[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:

$$\int_{\mathbb{R}^{R}}^{\mathbb{R}} \frac{dr}{r^{2} - 2ar + 1} = S \int_{0}^{\mathbb{R}} dx.$$
[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 $\frac{1}{r^2 - 2ar + 1} = \frac{A}{\left(r - a - \sqrt{a^2 - 1}\right)} + \frac{B}{\left(r - a + \sqrt{a^2 - 1}\right)}$
Putting the RHS over a common denominato r yields:

$$A\left(r - a + \sqrt{a^2 - 1}\right) + B\left(r - a - \sqrt{a^2 - 1}\right) = 1.$$

$$A + B = 0.$$
 [6]

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

$$A = \frac{1}{2\sqrt{a^2 - 1}}.$$

Equation [5] becomes:

$$\int_{R'}^{R} \frac{1}{r - a - \sqrt{a^2 - 1}} - \frac{1}{r - a + \sqrt{a^2 - 1}} dr = 2\sqrt{a^2 - 1} S \int_{0}^{X} dx$$
 and,
$$\left[\ln \left\{ \frac{r - a - \sqrt{a^2 - 1}}{r - a + \sqrt{a^2 - 1}} \right\} \right]_{R'}^{R} = 2\sqrt{a^2 - 1} S X,$$

$$\ln \left[\frac{R - a - \sqrt{a^2 - 1}}{R - a + \sqrt{a^2 - 1}} \bullet \frac{R' - a + \sqrt{a^2 - 1}}{R' - a - \sqrt{a^2 - 1}} \right] = 2\sqrt{a^2 - 1} S X.$$
 It is usual to substitute
$$b = \sqrt{a^2 - 1}$$
 giving
$$\ln \left[\frac{R - a - b}{R - a + b} \bullet \frac{R' - a + b}{R' - a - b} \right] = 2bSX$$

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 ∞ , which means that the denominator must equal 0 and:

$$R_{\infty} = a - \sqrt{a^2 - 1}$$

$$= 1 + \frac{K}{S} - \sqrt{\frac{K^2}{S^2} + \frac{2K}{S}}.$$
[9]

[7]

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

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

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

$$= \frac{1}{2R_{\infty}} \sqrt{R_{\infty}^4 - 2R_{\infty}^2 + 1}$$
 and, by convention , $b = \frac{1 - R_{\infty}^2}{2R}$.

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

$$SX = \frac{R_{\omega}}{1 - R_{\omega}^{2}} \ln \left[\frac{\left(R' - R_{\omega}\right) \left(R - \frac{1}{R_{\omega}}\right)}{\left(R' - \frac{1}{R_{\omega}}\right) \left(R - R_{\omega}\right)} \right]$$
[11]

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 $< 2 \text{ m}^2 \text{ kg}^{\text{-1}}$ for coated and uncoated fine papers made from bleached chemical pulps, is $3 < k < 6 \text{ m}^2 \text{ kg}^{\text{-1}}$ for mechanical pulps and is around $14 \text{ m}^2 \text{ kg}^{\text{-1}}$ for unbleached kraft pulps.

s is $> 50 \text{ m}^2 \text{ kg}^{-1}$ for filled and coated fine papers, $20 < s < 40 \text{ m}^2 \text{ kg}^{-1}$ for bleached and unbleached chemical pulps and is typically $40 < s < 70 \text{ m}^2 \text{ kg}^{-1}$ 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]:

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

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

Re arranging:

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

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

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

Opacity =
$$\frac{R_0}{R_m}$$

 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:

$$s = \frac{1}{W} \left(\frac{R_{\omega}}{1 - R_{\omega}^{2}} \right) \ln \left\{ R_{\omega}^{2} \frac{R_{0} - \frac{1}{R_{\omega}}}{R_{0} - R_{\omega}} \right\}$$
[13]

Now, using equation [12], R₀ for the standard grammage, W_{std} can be calculated:

$$R_{0} = \frac{\exp\left\{\left(\frac{1}{R_{\omega}} - R_{\omega}\right) s W_{std}\right\} - 1}{\frac{1}{R_{\omega}} \exp\left\{\left(\frac{1}{R_{\omega}} - R_{\omega}\right) s W_{std}\right\} - R_{\omega}}.$$
[14]