FABRIC COLOR FORMULATION USING A MODIFIED KUBELKA-MUNK THEORY CONSIDERING THERMAL EFFECT

by

Ling LIN^{a,b*} and Ling ZHAO^{a,b*}

^a Zhejiang Fashion Institute of Technology, Ningbo, China ^b Qingdao Product Quality Testing Research Institute, Qingdao, China

> Original scientific paper https://doi.org/10.2298/TSCI2303811L

The Kubelka-Munk function is simple but it ignores the film's thickness, so its applications are greatly limited. Though the exact relationship between the Kubelka-Munk function and the thickness can be derived from a differential model, it is too complex to be practically used. Here a modification is suggested by taking the thickness effect and the temperature effect into account, and the validity is widely enlarged. The modified Kubelka-Munk theory can be used as a colormatching model for colorful fabrics. If the porosity of the film is considered, a fractal modification with two-scale fractal derivative has to be adopted.

Key words: optical property, colorful fabrics, absorption coefficient, scattering coefficient, homotopy matching, porous film, two-scale fractal

Introduction

Colorful fabrics are widely used in textile engineering, especially the photochromic fabrics [1, 2] and thermochromic fabrics [3, 4] are the most used intelligent materials, and chameleon fabrics [5, 6] have been catching a rocketing interest in various fields from responsive camouflage to brand protection. Colorful fabrics can be also used as sensors [7] far behind fashion apparel, and far-reaching implications are emerging for applications including radiation protection [8] and energy harvesting [9]. Now the nanodyeing technology [10] has been making colorful fabrics extremely promising and remarkably challenging.

The Kubelka-Munk theory is widely used in textile engineering to describe light scattering and absorption of optical behavior of a fabric, it was first proposed by Franz Munk and Franz Munk in 1931 [11]. The Kubelka-Munk function is the main tool to fabric color formulation, it can be written in the form [11]:

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

where K and S are the absorption coefficient and the scattering coefficient of the fabric, respectively, and R is the reflectance.

Equation (1) is the famous equation for light absorption and scattering through a paint layer. It was derived under the assumption of infinite thickness $(L \rightarrow \infty)$, though many

^{*} Corespondings authors, e-mail: linling81@163.com, zhaolingyy@aliyun.com

experiment showed that when L > 2 mm, eq. (1) can be used with relatively high accuracy [12]. The Kubelka-Munk theory is the basic tool in color matching technology [13-20], it has been caught much attention in different fields, *e.g.*, textile engineering, material science, physics and chemistry. Though there were claims on misuse of the Kubelka-Munk function [16] and many modified Kubelka-Munk functions were appeared in open literature, mathematical treatment on the original Kubelka-Munk theory was rare.

When the substrate is extremely thin (L <<1), for examples, micro fibers [21], nanoscale membranes [22, 23], eq. (1) leads to a large error, this is because K/S depends upon L, and there is a significant flaw to apply eq. (1) to films with nano/micro thickness [16-18].

The optical properties of biological tissues are extremely special at 633 nm [24], when the thickness reduces to about 220 nm, as that in the nanostructure optical surface of the moth eyes [25], eq. (1) becomes totally invalid. Now the electrospinning or the bubble electrospinning [26-30] can produce thin films with thickness of about 100 nm, and the nanodyeing [10] also asks for a modified Kubelka-Munk function.

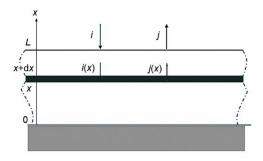


Figure 1. Kubelka-Munk model for color formulation

Kubelka-Munk theory

Kubelka and Munk established a differential model to study the change of incident light intensity travelling downwards, i, and upwards, j, within a thin film [11], fig. 1. The changes of i and j through an infinite distance, dx, are, respectively [11]:

$$di = -[-(K+S)i + Sj]dx$$
(2)

and

$$dj = [-(K+S)j + Si]dx$$
(3)

where *S* is the absorption coefficient, and *K* the scattering coefficient. From eqs. (2) and (3), we have:

$$\frac{\mathrm{d}j}{j} - \frac{\mathrm{d}i}{i} = -2(K+S)\mathrm{d}x + S\left(\frac{i}{j} + \frac{j}{i}\right)\mathrm{d}x \tag{4}$$

The reflectance is:

$$r = \frac{j}{i} \tag{5}$$

Equation (4) becomes:

$$d\ln r = -2(K+S)dx + S\left(r + \frac{1}{r}\right)dx$$
(6)

Solving eq. (6) exactly, we have:

$$\frac{1}{2\sqrt{\lambda^2 - 1}} \ln \left[\frac{\left(R_s - \lambda + \sqrt{\lambda^2 - 1}\right) \left(R - \lambda - \sqrt{\lambda^2 - 1}\right)}{\left(R - \lambda + \sqrt{\lambda^2 - 1}\right) \left(R_s - \lambda - \sqrt{\lambda^2 - 1}\right)} \right] = SL$$
(7)

where $\lambda = (K/S) + 1$, R_s is the reflectance when L = 0. Equation (7) is too complex to be used for practical applications. When $L \to \infty$, from eq. (7) we have:

$$\left(R - \lambda + \sqrt{\lambda^2 - 1}\right)\left(R_s - \lambda - \sqrt{\lambda^2 - 1}\right) = 0$$
(8)

or

$$R - \left(\frac{K}{S} + 1\right) + \sqrt{\left(\frac{K}{S} + 1\right)^2 - 1} = 0 \tag{9}$$

or

$$\left(R - \frac{K}{S} + 1\right)^2 = \left(\frac{K}{S} + 1\right)^2 - 1 \tag{10}$$

Solving K/S from eq. (10), we have eq. (1), so mathematically eq. (1) is valid only for $L \to \infty$.

Modified Kubelka-Munk function

We consider another case when $r \ll 1$. Under this assumption, we have:

$$r + \frac{1}{r} \approx \frac{1}{r} \tag{11}$$

Equation (6) becomes:

$$dr = -2(K+S)rdx + Sdx$$
(12)

or

$$\frac{\mathrm{d}r}{-2(K+S)r+S} = \mathrm{d}x\tag{13}$$

or

$$d\left\{\frac{\ln[-2(K+S)r+S]}{-2(K+S)}\right\} = dx$$
(14)

Solving eq. (14) gives the following result:

$$\frac{\ln[S - 2(K+S)R_s] - \ln[S - 2(K+S)R]}{-2(K+S)} = L$$
(15)

or

$$\ln\left[1-2\left(\frac{K}{S}+1\right)R_{s}\right] - \ln\left[1-2\left(\frac{K}{S}+1\right)R_{s}\right] = -2\left(\frac{K}{S}+1\right)SL$$
(16)

This simplified one is valid for small R, that is for the case with little scattering. Equation (16) has some potential applications to the color matching of micro/nanofibers with low scattering coefficient.

Another Modified Kubelka-Munk function

Consider the following inequality:

$$r + \frac{1}{r} \ge 2 \tag{17}$$

Equation (6) becomes a simple relation, which reads [2]:

$$d\ln r = -2(K+S)dx + S\left(r + \frac{1}{r}\right)dx \ge -2(K+S)dx + 2Sdx = -2Kdx$$
(18)

That means:

$$\ln\left(\frac{R}{R_s}\right) \ge -2\frac{K}{S}SL \tag{19}$$

or

$$\frac{K}{S} \ge -\frac{1}{2SL} (\ln R - \ln R_s) \tag{20}$$

Considering eq. (1) and eq. (20), we modify the Kubelka-Munk function:

$$\frac{K}{S} = \frac{\alpha(L)(1-R)^2}{2R} + \frac{1-\alpha(L)}{2SL}(\ln R_s - \ln R)$$
(21)

where α is a matching parameter, it is a function of *L*, it requires $\alpha(L > 2 \text{ mm}) = 1$ and $\alpha(L=0) = 0$. We call eq. (21) the homotopy matching, when $\alpha = 0$, it becomes eq. (21), and when $\alpha = 1$, it turns out to be eq. (1). The homotopy matching is widely applied in mathematics to solve non-linear problems [31, 32].

We choose the matching parameter as:

Lin, L., *et al.*: Fabric Color Formulation Using a Modified Kubelka-Munk Theory ... THERMAL SCIENCE: Year 2023, Vol. 27, No. 3A, pp. 1811-1818

$$\alpha = (1 - \mathrm{e}^{-aL})^b \tag{22}$$

1815

where a and b are parameters for experimental determination. eq. (21) becomes:

$$\frac{K}{S} = \frac{(1 - e^{-aL})^b (1 - R)^2}{2R} + \frac{[1 - (1 - e^{-aL})^b]}{2SL} (\ln R_s - \ln R)$$
(23)

It is well known that reflectance is temperature-dependent [33]. If the thermal effect is considered, eq. (23) can be modified:

$$\frac{K}{S} = \frac{\{1 - [1 - (1 - e^{-aL})^b]^c\}(1 - R)^2}{2R} + \frac{[1 - (1 - e^{-aL})^b]^c}{2SL}(\ln R_s - \ln R)$$
(24)

where c is a temperature-dependent parameter.

For multiple constituents, the above equation can be modified:

$$\frac{\sum_{i=1}^{N} K_i}{\sum_{i=1}^{N} S_i} = \frac{\{1 - [1 - (1 - e^{-aL})^b]^c\}(1 - R)^2}{2R} + \frac{[1 - (1 - e^{-aL})^b]^c}{2SL}(\ln R_s - \ln R)$$
(25)

where N is the number of constituents, for examples, when a fabric is coated by TiO₂ film, K_i (i = 1, 2) and S_i (i = 1, 2) are the absorption coefficient and the scattering coefficient for the fabric and TiO₂ film, respectively.

Discussion and conclusions

N

When we consider the porosity of the film, a fractal modification of the Kubelka-Munk function is needed. Eqs. (2) and (3) has to be modified:

$$di = -[-(K+S)i + Sj]dx^{\beta}$$
(26)

and

$$dj = [-(K+S)j + Si]dx^{\beta}$$
(27)

where β is the fractal dimensions of the film. The two-scale fractal derivative is [34-36]:

$$\frac{\mathrm{d}i}{\mathrm{d}x^{\beta}}(x_0) = \Gamma(1+\beta) \lim_{\substack{x-x_0 \to \Delta x \\ \Delta x \neq 0}} \frac{i(x) - i(x_0)}{(x-x_0)^{\beta}}$$
(28)

$$\frac{dj}{dx^{\beta}}(x_{0}) = \Gamma(1+\beta) \lim_{\substack{x-x_{0} \to \Delta x \\ \Delta x \neq 0}} \frac{j(x) - j(x_{0})}{(x-x_{0})^{\beta}}$$
(29)

where Γ is the gamma function. The two-scale fractal theory is now widely applied for porous problems, see for examples, the fractal diffusion [37], the fractal solitary wave [38], the fractal micro-electro-mechanical devices [39], the fractal concrete [40-43], and the fractal composite [44].

By a similar operation as previous, eq. (6) becomes:

$$d\ln r = -2(K+S)dx^{\beta} + S\left(r+\frac{1}{r}\right)dx^{\beta}$$
(30)

The solution of eq. (30) reads:

$$\frac{1}{2\sqrt{\lambda^2 - 1}} \ln \left[\frac{\left(R_s - \lambda + \sqrt{\lambda^2 - 1}\right) \left(R - \lambda - \sqrt{\lambda^2 - 1}\right)}{\left(R - \lambda + \sqrt{\lambda^2 - 1}\right) \left(R_s - \lambda - \sqrt{\lambda^2 - 1}\right)} \right] = SL^{\beta}$$
(31)

We will further discuss this fractal model in a forthcoming article.

To be concluded, this paper suggests a modified Kubelka-Munk function, eq. (24), which is also simple and considers the thickness of the film and temperature-dependent reflectance. If the porosity of the film is considered, the two-scale fractal modification is a must.

The parameters a and b and c involved in eq. (24) can be estimated experimentally. The modified Kubelka-Munk function can be used for a color-matching model for colorful fabrics, and far-reaching implications are emerging for applications include colorful image technology [45, 46] and microelectromechanical systems [47, 48].

References

- Cheng, T., et al., Photochromic Wool Fabrics from a Hybrid Silica Coating, *Textile Research Journal*, 77 (2007), 12, pp. 923-928
- [2] Cheng, T., et al., Fast Response Photochromic Textiles from Hybrid Silica Surface Coating, Fibers and Polymers, 9 (2008), 3, pp. 301-306
- [3] Yang, M. Y., et al., CNT/Cotton Composite Yarn for Electro-Thermochromic Textiles, Smart Materials and Structures, 28 (2019), Aug., 085003
- [4] Civan, L., Kurama, S., A Review: Preparation of Functionalised Materials/Smart Fabrics that Exhibit Thermochromic Behaviour, *Materials Science and Technology*, *37* (2021), 18, pp. 1405-1420
- [5] Ghosh, S., et al., Study of Chameleon Nylon and Polyester Fabrics Using Photochromic Ink, Journal of the Textile Institute, 109 (2018), 6, pp. 723-729
- [6] Hardaker, S. S., Gregory, R. V., Progress Toward Dynamic Color-Responsive "Chameleon" Fiber Systems, *MRS Bulletin*, 28 (2003), 8, pp. 564-567
- [7] Tang, Y., et al., Colorful Conductive Threads for Wearable Electronics: Transparent Cu-Ag Nanonets, Advanced Science, 9 (2022), 24, 2201111
- [8] He, J. H., et al., Review on Fiber Morphology Obtained by Bubble Electrospinning and Blown Bubble Spinning, *Thermal Science*, 16 (2013), 5, pp. 1263-1279
- [9] Wang, Q. L., et al., Intelligent Nanomaterials for Solar Energy Harvesting: From Polar Bear Hairs to Unsmooth Nanofiber Fabrication, Frontiers in Bioengineering and Biotechnology, 10 (2022), July, 926253
- [10] Ning, C. J., et al., Nano-Dyeing, Thermal Science, 20 (2016), 3, pp. 1003-1005
- [11] Kubelka, P., Munk, F., Ein Beitrag Zur Optik Der Farbanstriche, Z. Techn. Phys., 12 (1931), Aug., pp. 593-601
- [12] Escobedo-Morales, A., et al., Automated Method for the Determination of the Band Gap Energy of Pure and using diffuse reflectance Mixed Powder Samples Spectroscopy, *Heliyon*, 5 (2019), 4, e01505
- [13] Shen, J., et al., On the Kubelka-Munk Absorption Coefficient, Dyes Pigments, 127 (2016), Apr., pp. 187-188
- [14] Nakamura, D. M., et al., Color Formulation in Maxillofacial Elastomer by Genetic Algorithm, Dyes Pigments, 196 (2021), Dec., 109820
- [15] Soliman, H. N., Yahia, I. S., Synthesis and Technical Analysis of 6-Butyl-3-[(4-Chlorophenyl)Diazenyl]-4-Hydroxy-2H-Pyrano[3,2-c] Quinoline-2,5(6H)-Dione as A New Organic Semiconductor: Structural, Optical and Electronic Properties, *Dyes Pigments*, 176 (2020), 108199
- [16] Landi, S., et al., Use and Misuse of the Kubelka-Munk Function to Obtain The Band Gap Energy from Diffuse Reflectance Measurements, Solid State Commun., 341 (2022), Jan., 114573

- [17] Chen, H., et al., Full Solar-Spectral Reflectance of ZnO QDs/SiO2 Composite Pigment for Thermal Control Coating, Mater. Res. Bull., 146 (2022), Feb., 111572
- [18] Sochorova, S., Jamriska, O., Practical Pigment Mixing for Digital Painting, ACM T, Graphic, 40 (2021), 6, 234
- [19] Yang, R. H., et al., Color-Matching Model of Digital Rotor Spinning Viscose Melange Yarn Based on the Kubelka-Munk Theory, *Textile Research Journal*, 92 (2022), 3-4, pp. 574-584
- [20] Moussa, A., Textile Color Formulation Using Linear Programming Based on Kubelka-Munk and Duncan Theories, *Color Research and Application*, 46 (2021), 5, pp. 1046-1056
- [21] Doan, H. N., et al., Fabrication and Photochromic Properties of Force Spinning (R) Fibers Based on Spiropyran-Doped Poly(Methyl Methacrylate), RSC Advances, 7 (2017), 53, pp. 33061-33067
- [22] He, J. H., et al. The Maximal Wrinkle Angle During the Bubble Collapse and Its Application to the Bubble Electrospinning, Frontiers in Materials, 8 (2022), Feb., 800567
- [23] Qian, M. Y., He, J. H., Collection of Polymer Bubble as a Nanoscale Membrane, Surfaces and Interface, 28 (2022), Feb., 101665
- [24] Cheong, W. F., et al., A Review of the Optical-Properties of Biolodical Tissues, IEEE J. Quantum Elect., 26 (1990), 12, pp. 2166-2185
- [25] Muniraju, C. B., et al., Modeling of Enhancement Effect of Moth-Eye Antireflective Coating on Organic Light-Emitting Diode, J. Nanophotonics, 12 (2018), 4, 046021
- [26] Li, X. X., He, J. H., Bubble Electrospinning with an Auxiliary Electrode and an Auxiliary Air Flow, *Recent Patents on Nanotechnology*, 14 (2020), 1, pp. 42-45
- [27] Liu, L. G., et al., Dropping in Electrospinning Process: A General Strategy for Fabrication of Microspheres, *Thermal Science*, 25 (2021), 2, pp. 1295-1303
- [28] Lin, L., et al., Fabrication of PVDF/PES Nanofibers with Unsmooth Fractal Surfaces by Electrospinning: A General Strategy and Formation Mechanism, *Thermal Science*, 25 (2021), 2, pp. 1287-1294
- [29] Tian, D., He, C. H., From Inner Topological Structure to Functional Nanofibers: Theoretical Analysis and Experimental Verification, *Membranes*, 11 (2021), 11, 870
- [30] Tian, D., He, J. H., Macromolecular-Scale Electrospinning: Controlling Inner Topologic Structure Through a Blowing Air, *Thermal Science*, 26 (2022), 3B, pp. 2663-2666
- [31] He, C. H., El-Dib, Y. O., A Heuristic Review on the Homotopy Perturbation Method for Non-Conservative Oscillators, J. Low Freq. Noise V. A., 41 (2022), 2, pp. 572-6032021
- [32] Li, X. X., He, C. H., Homotopy Perturbation Method Coupled with the Enhanced Perturbation Method, J. Low Freq. Noise V. A., 38 (2019), 3-4, pp. 1399-1403
- [33] Michael, C., et al., Supercontinuum-Laser Diffuse Reflectance Spectroscopy in conjunction with an extended Kubelka-Munk model-a Methodology for Determination of Temperature-Dependent Quantum Efficiency in Highly Scattering and Fluorescent Media, Appl. Opt., 58 (2019), 10, pp. 2438-2445
- [34] He, J. H., When Mathematics Meets Thermal Science, The Simpler is the Better, *Thermal Science*, 25 (2021), 3B, pp. 2039-2042
- [35] He, J. H., Seeing with a Single Scale is Always Unbelieving: From Magic to Two-Scale Fractal, *Ther-mal Science*, 25 (2021), 2B, pp. 1217-1219
- [36] Qian, M. Y., He, J. H., Two-Scale Thermal Science for Modern Life –Making the Impossible Possible, *Thermal Science*, 26 (2022), 3B, pp. 2409-2412
- [37] He, J. H., Qian, M. Y., A Fractal Approach to the Diffusion Process of Red Ink in A Saline Water, *Thermal Science*, 26 (2022), 3B, pp. 2447-2451
- [38] Wu, P. X., et al., Solitary Waves of the Variant Boussinesq-Burgers Equation in a Fractal Dimensional Space, Fractals, 30 (2022), 3, 2250056
- [39] He, C. H., A Variational Principle for a Fractal Nano/Microelectromechanical (N/MEMS) System, International Journal of Numerical Methods for Heat & Fluid Flow, 33 (2022), 1, pp. 351-359
- [40] He, C. H., Liu, C., Fractal Approach to the Fluidity of a Cement Mortar, Non-linear Engineering, 11 (2022), 1, pp. 1-5
- [41] He, C.-H., et al., A Fractal Model for the Internal Temperature Response of a Porous Concrete, Applied and Computational Mathematics, 21 (2022), 1, pp. 71-77
- [42] He, C. H., et al., A Novel Bond Stress-Slip Model for 3-D Printed Concretes, Discrete and Continuous dynamical Systems, 15 (2022), 7, pp. 1669-1683
- [43] He, C. H., Liu, C., A Modified Frequency-Amplitude Formulation for Fractal Vibration Systems, Fractals, 30 (2022), 3, 2250046

- [44] Zuo, Y.-T., Liu, H.-J., Fractal Approach to Mechanical and Electrical Properties of Graphene/Sic Composites, *Facta Universitatis-Series Mechanical Engineering*, *19* (2021), 2, pp. 271-284
 [45] Wang, S. Q., *et al.*, Prediction of Myelopathic Level in Cervical Spondylotic Myelopathy Using Diffu-
- [45] Wang, S. Q., et al., Prediction of Myelopathic Level in Cervical Spondylotic Myelopathy Using Diffusion Tensor Imaging, Journal of Magnetic Resonance Imaging, 41 (2015), 6, pp. 1682-1688
- [46] You, S. R., et al., Fine Perceptive GANS for Brain MR Image Super-Resolution In Wavelet Domain, IEEE Transactions on Neural Networks and Learning Systems, On-line first, https://doi.org/10.1109/ TNNLS.2022.3153088, 2022w
- [47] Saxena, N., *et al.*, Enhancement in Structural, Morphological and Optical Features of Thermally Annealed Zinc Oxide Nanofilm, *Indian Journal of Pure & Applied Physics*, 58 (2020), 8, pp. 642-648
- [48] Anjum, N., et al., Li-He's Modified Homotopy Perturbation Method for Doubly-Clamped Electrically Actuated Microbeams-Based Microelectromechanical System, Facta Universitatis Series: Mechanical Engineering, 19 (2021), 4, pp. 601-612