Research Square

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Optical properties in the visible range of two different India ink used as biological phantoms

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Research

Keywords: Parker ink, Pelikan ink, Albedo, Absorption coefficient, Integrating sphere

DOI: https://doi.org/10.21203/rs.3.rs-28606/v1

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Abstract

The optical characteristics of two different brands of India ink, Parker Quink and Pelikan, as an absorber used in preparation a tissue-simulating phantom, have been investigated at visible wavelength range. For this purpose, a single integrating sphere system and a spectrophotometric transmission spectroscopy have been used to estimate the radiometric characteristics. Then, inverse adding-doubling algorithm was implemented to retrieve the optical coefficients of pure ink samples. Parker ink's absorption behavior turned out to incompatible with Pelikan over the present wavelength range. Furthermore, scattering property of both two brands has been exhibited and the albedo was calculated. Parker albedo showed a decremental behavior with wavelength and varied between 0.381 and 0.13. A structural profile of albedo was found for Pelikan, which varied between 0.366 and 0.03. This discrepancy might be explained by the variety of two brands composition besides experimental errors. Furthermore, Parker ink absorption variation turned out to be in correspondence to several tissues' absorption feature over broad wavelength ranges. Finally, Parker ink could be regarded as a better candidate to mimic absorption property for several tissues.

Introduction

In recent decades, optical methods have become widely used in biomedical diagnostics and therapies because of the applicability of light to non-destructively penetrate into a tissue. To evaluate techniques, calibrate equipment, optimize procedures and test theoretical predictions experimentally, optical tissue phantoms have been required [1–4]. Since biological tissues are turbid media, optical phantoms should include scattering and absorbing materials to simulate tissue's optical properties [1–4]. India ink has been commonly used as an absorber in optical phantom manufacturing [1–8]. The reason for widespread uses of India ink is that ink has many advantages. The main advantages are that it is inexpensive, chemically and spectrally stable, nontoxic, and does not fluoresce [1–6]. However, the variety of commercial manufacturers and compositions are the main reason of their optical characteristics variation. Furthermore, all prior research groups that aimed to characterize the optical properties of India ink, showed the possibility of inter-brand and inter-batch variations as well as the existence of ink scattering property [5–8]. *Madeson et al* investigated deeply two different brands of ink (Higgins and Regal) and measured extinction coefficient, anisotropy factor and albedo of these samples via spectral characteristics [5]. All measurement were carried out at 594 nm. The scattering coefficient had been obtained and the albedo of these samples was 0.29 and 0.43 besides to inter-brand and inter-batch variations [5]. Martelli and Zaccanti also estimated absorption coefficient and albedo of Rotring ink at 750 nm. However, researchers investigated the scattering coefficient using calculating albedo that was about 0.125 [6]. Ninni et al. studied five different ink brands (Pelikan, Higgins, Rotring, Staedtler and Koh I Noor) at three wavelengths 632.8, 751 and 833 nm. The inter-brand and inter-batch optical characteristic varieties were obvious and the albedo was the largest value at 632.8 nm [7]. Accordingly, there are particular brands of India ink such as Pelikan, Rotring and Higgins that have been examined extensively and characterized optically [5–8]. However, black Parker Quink ink is composed of 48% carbon in the elementary state and 23% resinous and bituminous organic compound, in our knowledge, has not been characterized optically [9, 10]. Finally, there are several methods used to investigate the propagation of light in materials. Inverse adding-doubling algorithm has been regarded as a numerical solution of radiative transfer equation. To apply inverse adding-doubling method, three raw light intensities are required, total transmittance T, diffuse reflectance R_d and collimated transmittance T_c. This method repeatedly solves the radiative transfer equation until the solution and the measured values of radiometric characteristics be the same [11].

The aim of this research is to investigate the optical properties of two different India ink brands, Pelikan blue (D-30163 Hannover, Germany) and Parker black (1950375, United Kingdom). For this purpose, a single integrating sphere system and collimated transmission spectroscopy were used to extract extinction, absorption and scattering coefficients via radiometric characteristics and inverse adding-doubling algorithm [12]. Then, the results have been analyzed and discussed and advantages of using those brands have been presented.

Materials And Methods

Sample preparation

Generally, the pure optical properties of Parker black ink (1950375, United Kingdom) and Pelikan blue ink (D-30163 Hannover, Germany) have been determined by measuring the optical properties of dilutions that prepared with different volume concentrations of these two brands. Based on a linear relationship between optical coefficient and volume concentration, optical coefficients of pure ink (without dilution) could be extracted [7–9]. Accordingly, these two types of ink have been dissolved in distilled water to obtain two groups of sample with different volume concentrations. The first group of black ink has the volume concentrations (0.012, 0.02, 0.03, 0.06 and 0.09%) and the second group of blue ink has the concentrations (0.005, 0.008, 0.012, 0.016 and 0.022%).

Spectrophotometric transmission spectroscopy

A broad band, fiber based spectrophotometric transmission setup was arranged. It consists of broadband halogen–tungsten light source (HL-2000-HP-FHSA, Ocean Optics, USA), a fiber coupled cuvette holder with two collimating lenses (CUV-ATT-DA, Avantes, Netherlands), and a USB portable spectrometer (USB4000 FL, Ocean Optics, U.S.A.) [9, 13].

Single integrating sphere system

A broadband single integrating sphere (819C-IS-5.3, Newport, U.S.A.) system was assembled to measure diffuse reflectance R_d and total transmittance T. Figures (1) depicts diffuse reflection and total transmission measurement setups. Light from a tungsten-halogen source (HL-2000-HP-FHSA, Ocean Optics, U.S.A.) was focused via a convex lens (focal length, $\mathrm{f} = 10\mathrm{cm}$) to have a 5 mm spot diameter.

The diffuse light emanated from the sample is guided through an optical fiber (fiber diameter, $\varnothing = 400 \mu\mathrm{m}$) which connected to the spectrometer (USB4000 FL, Ocean Optics, U.S.A.) [13].

Results

Pelikan blue ink characterization

To retrieve the optical coefficients of blue ink, collimated transmittance T_c, diffuse reflectance R_d, and total transmittance T are needed. Figures (2-a) represents Pelikan blue ink's collimated (dashed), and total (solid) transmittances for all samples, which measured using spectrophotometric transmission spectroscopy and integrating sphere system respectively. Accordingly, transmittance was found to be inversely proportional to increased volume concentration as can be seen in Fig. (2-a). However, the existence of discrepancy between total transmittance and collimated transmittance refers to ink's scattering property, which could be predicted to be anisotropic. That might be proved by the diffuse reflectance spectrum of all samples, Fig. (2-b). Since the difference between total transmittance and collimated transmittance at every wavelengths exceeded the diffuse reflectance, forward scattering feature could be distinguished.

Based on spectrophotometric data and by applying inverse adding-doubling algorithm, the extinction, absorption and scattering coefficients of these diluted samples could be estimated [12]. Because of using low volume concentrations, optical coefficients of these diluted samples are linearly related to the volume concentrations of undiluted compounds. The relationship between absorption and extinction coefficients of Pelikan ink and volume concentration has been examined experimentally. Figures (3) presents the correlation of absorption and extinction of Pelikan and volume concentration at 632 nm respectively. Then, 343 mm^{-1} and 523.5 mm^{-1} can be considered as absorption and extinction coefficients of pure Pelikan sample at 632 nm respectively. Then, relative errors for absorption and extinction coefficients have been calculated to be 31.4% and 12.75% respectively [7, 8]. At this wavelength, albedo value was approximately 0.344 that is larger than the predicted value. Then, pure optical coefficients of two ink brands (without dilution) over the present wavelength range could be measured.

Figure (4-a) depicts extinction coefficient (solid) for Pelikan ink with wavelength that shows a similar trend in comparison to a prior work over the presented wavelength range [14]. Then, absorption coefficient of pure Pelikan sample (dashed line) has a structural behavior with wavelength. That varied between 61 mm^{-1} at 675 nm and 430 mm^{-1} at 616 nm, as shown in Fig. (4-a). Furthermore, Pelikan absorption coefficient turned out to be progressively proportional to increased wavelength over the sub-range varied from 500 nm to 616 nm and inversely proportional to increased wavelength over the rest of wavelength range. Figures (4-a) depicts Pelikan scattering coefficient (dotted line), which varied between 243 mm^{-1} at 616 nm and 2 mm^{-1} at 675 nm. Accordingly, correlation of scattering coefficient with wavelength has a similar profile in comparison to absorption coefficient besides to the existence of quantitative disagreement. Finally, based on blue ink absorption and scattering coefficients, their albedo could be predicted and its correlation with wavelength found to be structural as can be shown in Fig. (4-b).

Parker black ink characterization

Depending on spectrophotometric transmission spectroscopy and integrating sphere system, spectroscopic characteristics for black ink samples could be evaluated. Figures (5-a) presents collimated (dashed) and total (solid) transmittance of Parker ink over the present wavelength range. Parker diffuse reflectance spectra could be seen in Fig. (5-b). As mentioned above, the differences between collimated and total transmittance besides to diffuse reflectance can be considered as an improvement of black ink scattering property.

Depending on spectrophotometric measurements of black ink samples and inverse adding-doubling algorithm, optical coefficients could be expected for all samples at all wavelengths. Since using low volume concentrations, optical coefficients of these diluted samples are linearly related to the volume concentrations of undiluted compounds. Then, extinction, absorption and scattering coefficients for pure black ink could be retrieved. Figures (6-a) represents the relationship between pure absorption coefficient (dashed line) for Parker ink with wavelength, which ranged between 20 mm^{-1} at 675 nm and 217 mm^{-1} at 583 nm. For more details, absorption variation over the range of wavelength from 500 nm to 616 nm turned out to be more stable which varied between 154 mm^{-1} at 500 nm and 185 mm^{-1}at 616 nm and the maximum value was about 217 mm^{-1} at 583 nm. Dramatic changes of absorption could be seen at the rest of spectrum that were inversely proportional to increased wavelength, Fig. (6-a).

Parker scattering coefficient (dotted line) which expected previously, varied between 94.4 mm^{-1} at 500 nm and 5.2 mm^{-1} at 675 nm, as shown in Fig. (6-a). The scattering profile has a decremental behavior with wavelength unlike absorption correlation of black ink. Thus, albedo could be extracted using absorption and scattering coefficients that was found to be smoothly decreased with increased wavelength, Fig. (6-b). Qualitatively, black ink absorption profile has to be in accordance to some living tissues' absorption property but the quantitative dissimilarity can be distinguished. Figures (7-a) shows the relationship between absorption coefficient of adenocarcinoma and Parker ink with 0.23% volume concentration. It can be seen the correspondence of their absorption property especially over the sub-spectrum ranged from 500 nm to 580 nm. Absolute error varied between 0.0016 and 0.0836 after that the absolute error has increased dramatically which is obvious at Fig. (7-a) [15]. Figures (7-b) represents the absorption property of Parker ink with a 0.02% volume concentration in comparison to hemoglobin over the wavelength range varied between 600 nm to 670 nm. Although there is a discrepancy of absorption coefficient, absolute error could be evaluated to be 0.0035 at 630 nm and 0.002 at 650 nm [16]. Then, a relationship between Parker ink dilution with a 0.273% volume concentration and squamous cell carcinoma over a wide range varied from 500 nm to 580 nm has been shown, Fig. (7.c) [15]. Absolute error was found to be between 0.028 and 0.147.

Discussion

A spectrophotometric transmission spectroscopy and a single integrating sphere system were utilized to estimate spectrophotometric characteristics of these two groups of ink diluted samples. These considered as basic requirements to apply inverse adding-doubling algorithm for optical characterization. Furthermore, using a low concentration of dilution samples may predict pure optical coefficients of undiluted samples based on a linear relationship between coefficients and volume concentration. As can be seen from Figs. (4-a) and (6-a), Parker ink optical coefficients have different trends in comparison to Pelikan ink. Figures (4-a) depicts the correlation of absorption coefficient and wavelength of blue ink, that has a structural behavior. For shorter wavelengths, a direct relationship between absorption and wavelength could be shown. Then, over a wavelength spectrum ranged from 616 nm and 675 nm, an inverse relationship could be distinguished. Regarding the scattering coefficient that has a similar profile to the absorption property of blue ink, a quantitative disagreement could be shown. Generally, a single scattering approximation was mainly used to predict India ink scattering property [5–8]. Thus, a linear decremental behavior of ink scattering coefficient with wavelength has been applied. In that context, *Madeson et al* investigated the optical properties of India ink and clarified the possibility for aggregation of smaller carbon particles to form many different compositions with irregular shapes and dimensions [5]. Thus, scattering property of such media could not predicted previously but demands optical characterization. Accordingly, blue ink albedo could be calculated based on their optical coefficients, Fig. (4-b). Obviously, Pelikan albedo (dash-dotted) has a structured behavior and varied from 0.03 at 675 nm to 0.366 at 583 nm even more so it remained relatively stable over a sub-range from 533 nm to 637 nm around 0.3. Over that, Pelikan albedo decreased gradually with increased wavelength that to be in correspondence to the previous works [6–8]. All previous works aimed to retrieve the optical characteristics of Pelikan ink, carried out over the wavelength range above 594 nm. Over that range, a relative compatibility of albedo behavior could be recognized in which an inverse relationship with wavelength was shown. Furthermore, the differences of albedo values could be attributed to the scattering property discrepancy. That can be caused by the aggregation of smaller carbon particles that results in a variety of ink components' dimensions and shapes. Furthermore, the preparation of ink samples was not associated with ultrasound application that could prevent the aggregation of carbon particles. On the other hand, inter batch variation can cause a significant variability for optical characteristics that may affect albedo values [5, 7, 14].

On the other hand, Parker black ink absorption property has shown a stable relationship over the shorter wavelengths that varied from 500 nm to 616 nm. After that, an inverse correlation with wavelength could be observed. Scattering coefficient of black ink is inversely proportional to increased wavelength, Fig. (6-a). Thus, a large probability of attenuation photon with shorter wavelengths could be predicted, which could be noticed from transmission spectra. Furthermore, a decremental behavior of Parker scattering profile turned out to be in correspondence to the single scattering approximation. Furthermore, scattering profile may be considered as a median case between Ryleigh and Mie scatterings, which could be confirmed by a relative small dependency on wavelength that simulate a case between these limitations. However, the discrepancy between Pelikan and Parker scattering profile and the selective applicability of using that approximation for prediction could be returned to ink brand. In other words, the application of ultrasound before optical characterization is essential but depends on the ink brand and ingredients. Then, black ink coefficients could be used to estimate albedo values, Fig. (6-b). That showed a linear relationship with increased wavelength and ranged from 0.381 at 500 nm to 0.13 at 637 nm gradually. Thus, the behavior of Parker albedo with wavelength turned out to be in accordance to the literature despite a quantitative disagreement [7]. Quantitative variety could be explained by the irregularity of Parker ink ingredients and its disagreement compositions in comparison to other ink brands [5, 10]. To the best of our knowledge, Parker ink has not been examined for optical phantom construction. Although there is an incompatibility at the absorption spectrum of Parker ink, the behavior of absorption has been in agreement with cancerous stomach and esophagus besides hemoglobin absorption spectra over a wide wavelength range [15, 16]. Figures (7) represents comparing diluted ink samples' absorption property with these tissues. Otherwise, Pelikan absorption spectrum has different behavior in comparison to the previous tissues. Therefore, using Parker ink may be useful to simulate absorption property of some biological media and this compatibility can make Parker ink to be a better candidate in constructing optical phantoms [15, 16].

Conclusion

In summary, the results given in this paper were an attempt to investigate the optical properties of Parker and Pelikan inks as absorption components in solid and liquid optical phantoms. For this purpose, inverse adding-doubling algorithm was implemented to calculate their optical properties using radiometric characteristics. Finally, the results of measurements carried out on two different brands of ink showed:

- Significant differences of ink optical characteristics from batch to batch and brand to brand.
- Parker ink has small and more systematic variations of albedo in comparison to Pelikan ink.
- The necessity of optical characterization before using any batch of ink for constructing optical phantom. Because there is a significant variety of optical coefficients.
- Imperative need for ultrasound to prevent the aggregation that can cause a deviation in predicted optical coefficients.
- Parker ink can be more suitable to simulate some types of tissue over a wide wavelength range.

Declarations

Availability of data statement

The datasets generated and analysed during the current study are available from the corresponding author on reasonable request.

Competing interests

The authors declare that they have no competing interests.

Funding

The authors would like to thank Damascus University for its supports.

Authors contributions

The authors contributed equally to the paper.

Acknowledgments

The authors would like to thank all staff of biomedical photonics laboratory, Higher Institute for Laser Research and Applications, Damascus University.

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Figures

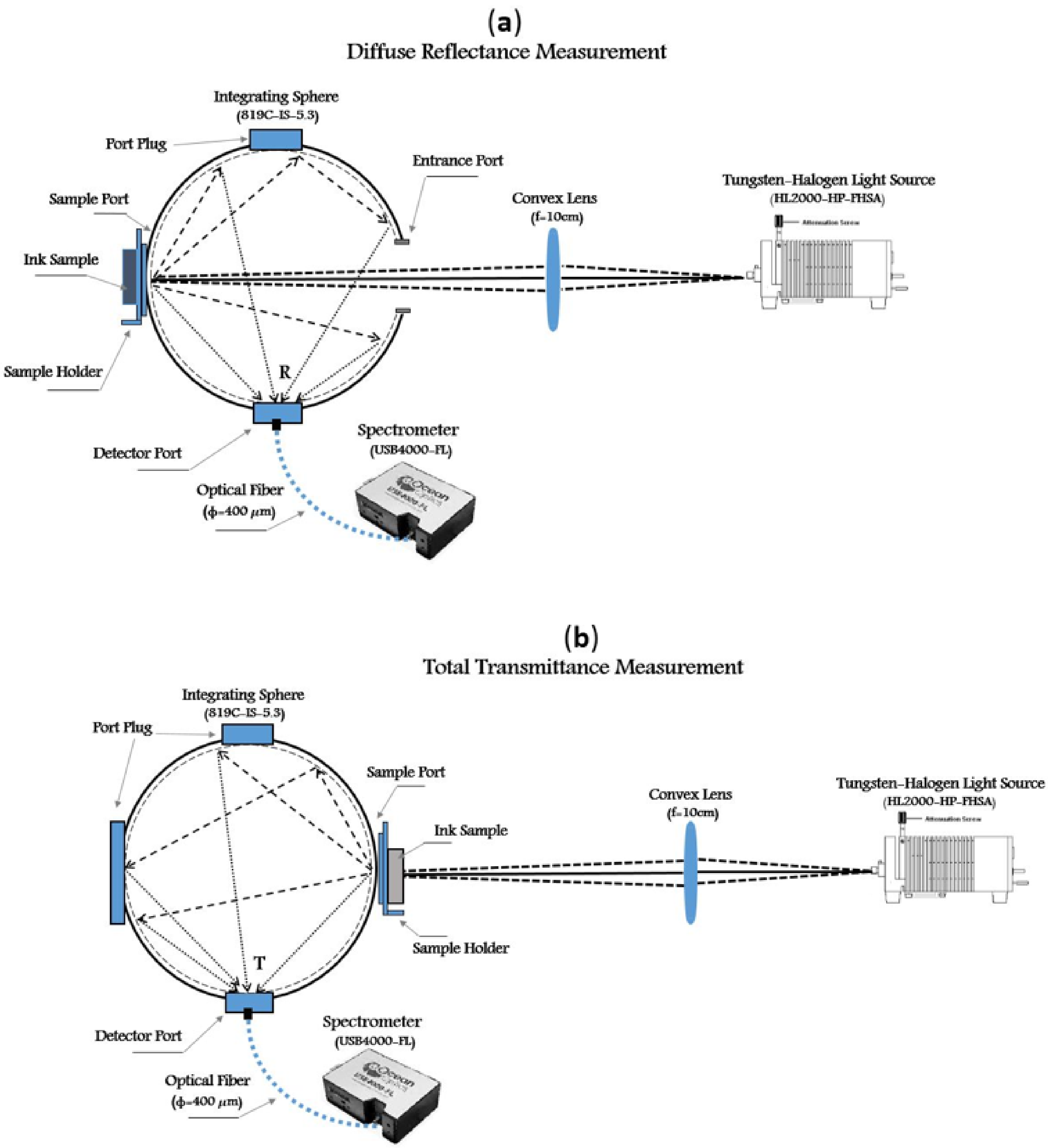

Figure 1

a): Schematic drawing of diffuse reflectance (Rd) measurement setup, tungsten-halogen light source was utilized to generate a focused beam using a convex lens (focal length, f=10cm). Then, ink sample illuminated via 4 mm spot light. Then, diffused light collected via an optical fiber (diameter, = 400 μm) that connected to spectrometer. b) Schematic drawing of total transmittance (T) measurement setup, tungsten-halogen light source was used to generate a focused beam using a convex lens (focal length, f=10cm). Then, ink sample was illuminated via 4 mm spot light diameter. Then, diffused light collected via an optical fiber (diameter, ▯ = 400 μm) that connected to spectrometer.

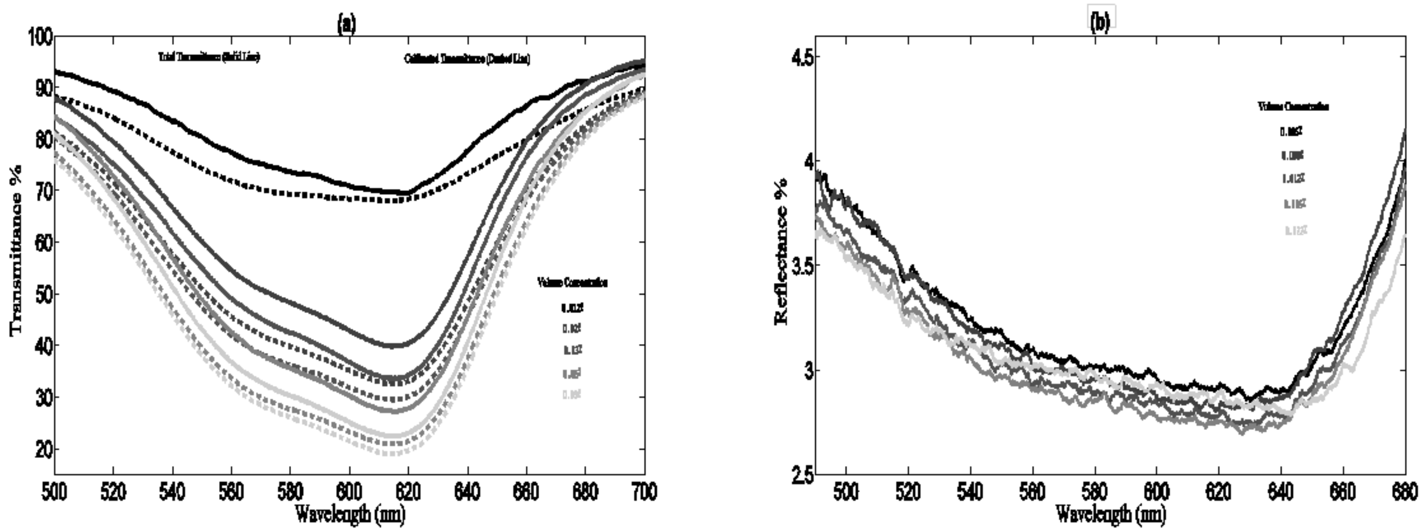

Figure 2

.a) Correlation of collimated transmittance (dashed) and total transmittance (solid) of Pelikan ink with wavelength for all samples, .b) Correlation of diffuse reflectance with wavelength of Pelikan ink for all samples.

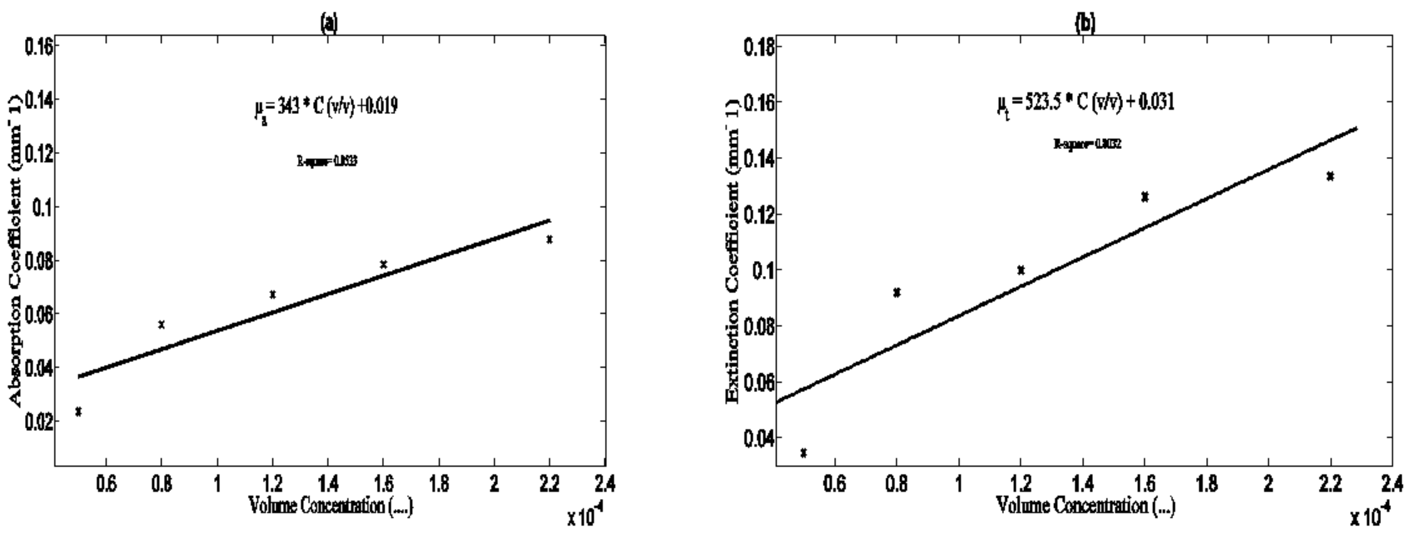

Figure 3

a) Correlation of blue ink absorption coefficient and volume concentration at 632nm, b) Correlation of extinction coefficient of Pelikan with concentration at 632nm.

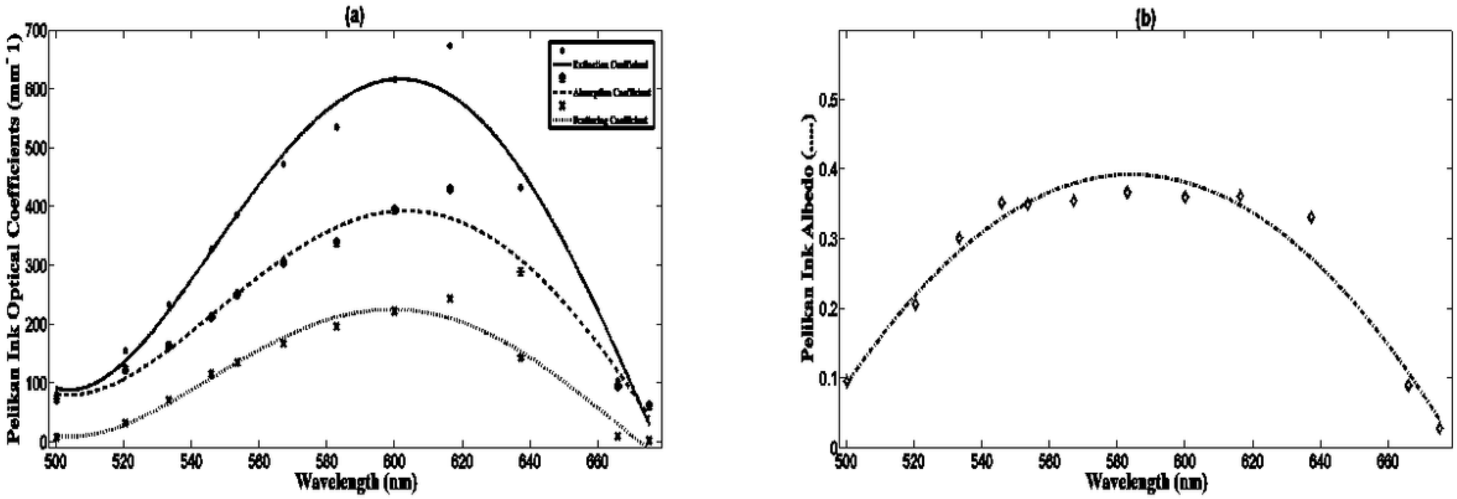

Figure 4

a) Relation between Pelikan optical properties, extinction (solid), absorption (dashed) and scattering (dotted), with wavelength, b) Pelikan ink's albedo variation over the wavelength range.

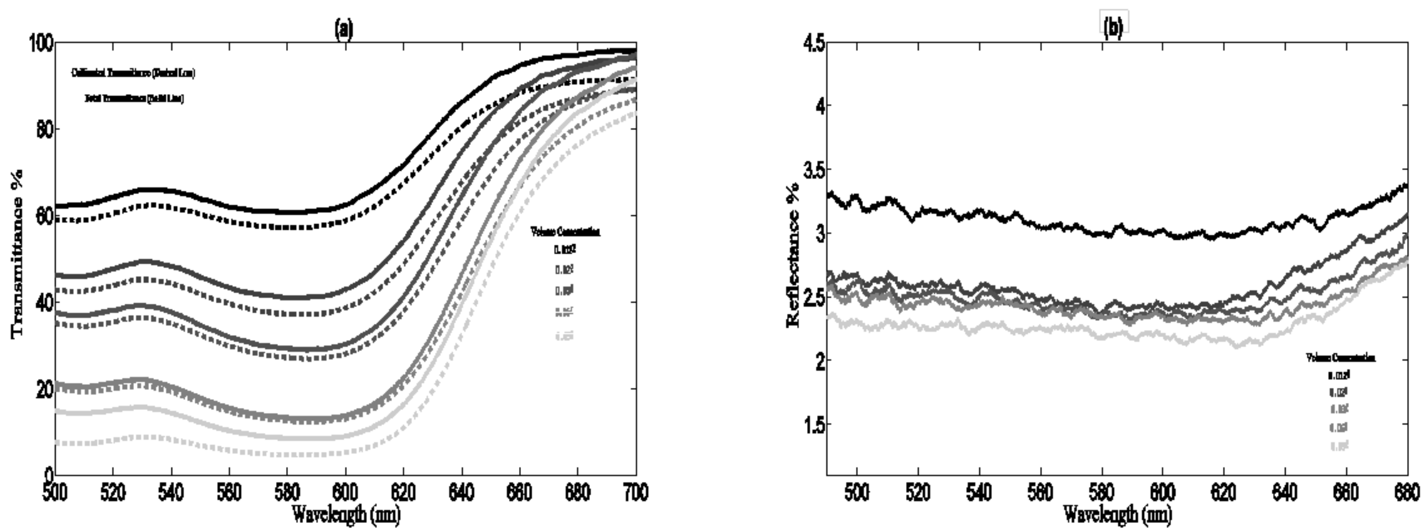

Figure 5

a) Correlation of collimated transmittance (dashed) and total transmittance (solid) of Parker ink samples with wavelength, .b) Correlation of diffuse reflectance with wavelength of Parker ink for all samples.

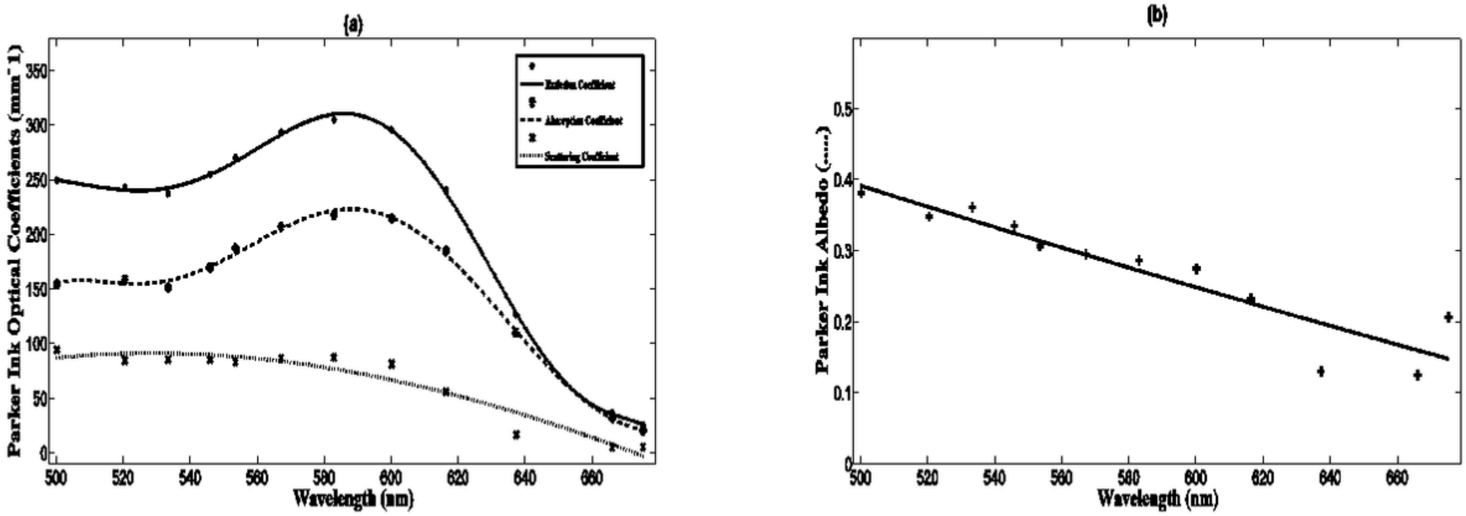

Figure 6

a) Relationship between Parker ink optical coefficients, extinction (solid), absorption (dashed) and scattering (dotted), with wavelength, b) Parker ink's albedo variation over the wavelength range.

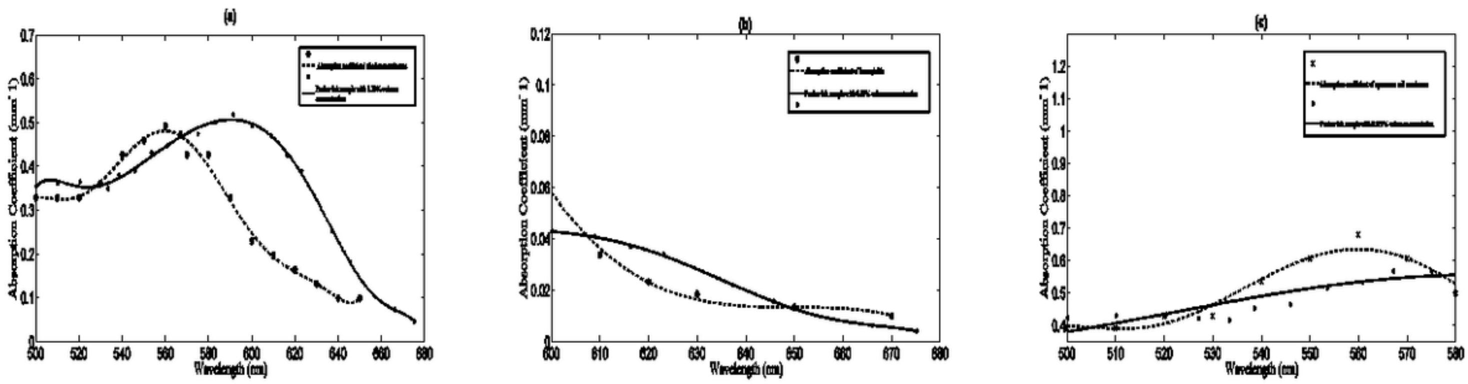

Figure 7

a) Comparison between Parker absorption coefficient (solid) with a 0.23% volume concentration with adenocarcinoma absorption coefficient (dashed line) over the present wavelength range, b) Comparison between 0.02% Parker absorption coefficient (solid) with hemoglobin (dashed) over a wavelength range 600 – 680nm, c) Relationship between absorption coefficient of squamous cell carcinoma (SSC) of esophagus and Parker (solid) sample with a 0.273% volume concentration over the present wavelength range.