

Polyurethane Phantoms with Homogeneous and Nearly Homogeneous Optical Properties

Ville T. Keränen^{ab}, Anssi J. Mäkynen^a, Amanda L. Dayton^b and Scott A. Prahl^b

^aUniversity of Oulu, Technology Park 127, Kajaani, Finland;

^bOregon Health and Science University, 9205 SW Barnes rd, Portland Oregon, USA

ABSTRACT

Phantoms with controlled optical properties are often used for calibration and standardization. The phantoms are typically prepared by adding absorbers and scatterers to a clear host material. It is usually assumed that the scatterers and absorbers are uniformly dispersed within the medium. To explore the effects of this assumption, we prepared paired sets of polyurethane phantoms (both with identical masses of absorber, India ink and scatterer, titanium dioxide). Polyurethane phantoms were made by mixing two polyurethane parts (a and b) together and letting them cure in a polypropylene container. The mixture was degassed before curing to ensure a sample without bubbles. The optical properties were controlled by mixing titanium dioxide or India ink into polyurethane part (a or b) before blending the parts together. By changing the mixing sequence, we could change the aggregation of the scattering and absorbing particles. Each set had one sample with homogeneously dispersed scatterers and absorbers, and a second sample with slightly aggregated scatterers or absorbers. We found that the measured transmittance could easily vary by a factor of twenty. The estimated optical properties (using the inverse adding-doubling method) indicate that when aggregation is present, the optical properties are no longer proportional to the concentrations of absorbers or scatterers.

Keywords: absorption, scattering, aggregation

1. INTRODUCTION

Phantoms with controlled optical properties are often used for calibration and standardization. The phantoms are typically prepared by adding absorbers and scatterers to a clear host material. It is usually assumed that the scatterers and absorbers are uniformly dispersed within the medium. To explore the effects of this assumption, we prepared paired sets of polyurethane phantoms (both with identical masses of absorber, India ink and scatterer, titanium dioxide).

2. PHANTOM PREPARATION

The polyurethane phantoms were made as described by Moffitt.¹ Polyurethane (WC-781, BJB Enterprises) was used as the host material. This polyurethane was chosen for its pot life (30 minutes) which gives sufficient time to mix the polyurethane, put it into molds, and degas. The short life also minimizes any settling of scatterers or absorbers added to the polyurethane. Titanium dioxide powder and India Ink (Speedball Inc) were used as scatterer and absorber respectively. Polyurethane by itself is a two component material that forms clear rigid blocks after curing. The basic manufacturing process is simple; part A and the part B are mixed together and then cured in a container. To ensure uniformity and reproducibility a few extra steps are required.

Further author information: (Send correspondence to V.K.)

V.K.: E-mail: ville.keranen@gmail.com, Telephone: +358 50 3277 811

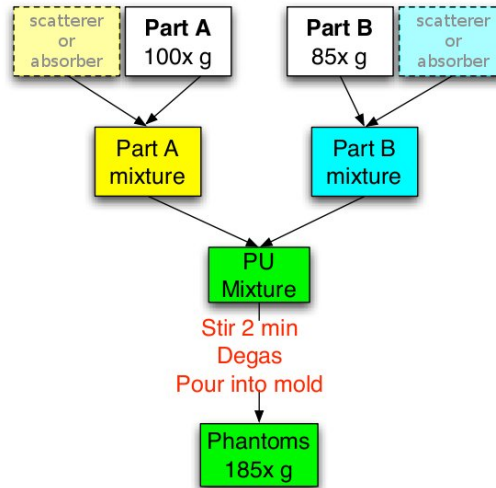


Figure 1. Phantom Flowchart

2.1 Mixing

Two sets of 2 samples were prepared. India ink or TiO_2 were mixed first with part A or part B and then with the other part (B or A). When ink or scatter is added to part B first, both disperse and mix well. However, when either is mixed with part A, although both appear to mix well, upon curing it is evident that aggregation of the scattering or absorbing particles occurs. Consequently, each set had one sample with homogeneously dispersed scatterers or absorbers, and a second sample with slightly aggregated scatterers or absorbers. The complete process is presented in Figure 1. India ink and TiO_2 stock solutions were prepared to make the amounts more accurate. To prepare the stock solutions 25 g of TiO_2 powder was mixed with 392 g (500 ml) of ethanol and 20 g of India ink was mixed with 180 g of ethanol. For each absorbing sample 365 μl of India ink stock solution was mixed with total 37 g of polyurethane. For each scattering sample 1510 μl of TiO_2 stock was mixed with total 37 g of polyurethane.

2.2 Degassing and curing

Part A and Part B were carefully mixed together and placed into a vacuum chamber to remove bubbles and dissolved air. The mixture bubbles vigorously at the beginning of the degassing cycle but the bubbling usually ends in less than 10 minutes. Since the pot time for this particular polyurethane is 30 minutes, it is possible to repeat the degassing process once to extract more bubbles. Samples cured in polypropylene containers (Nalgene 2116 Straight-Side Wide-Mouth Jar) produced solid phantoms with the clearest surfaces. Residual scattering by the surface is only an issue when tiny amounts of titanium oxide are added and the resulting sample is almost clear. Any scattering from the surface could be considered as scattering from the sample. As Moffitt has shown earlier¹ the polyurethane samples made this way are very consistent and stable.

3. MEASUREMENTS

Two methods were used to find differences between samples. All the samples were measured with integrating spheres and optical coefficients were calculated with inverse adding-doubling method. Pictures of the absorbing samples were taken with a light microscope. The pictures were taken to verify the aggregation.

3.1 Microscope Pictures

Each sample was put under the microscope and a picture was taken. The pictures of absorbing samples are presented in Figure 2. When the pictures are compared it is easy to see that the homogeneous sample on the left is homogeneous as the aggregated sample on the right has dark spots of India ink.

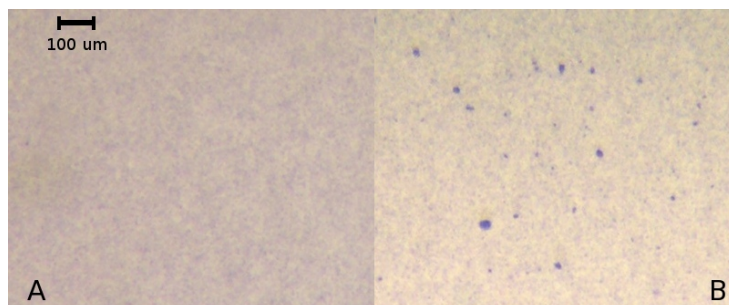


Figure 2. Homogeneous^A and aggregated^B India ink sample

3.2 Optical Properties

The optical properties of the samples were determined with integrating spheres and inverse adding-doubling method. Total diffuse reflection and transmission measurements were made using an 203.2 mm diameter integrating sphere (IS-080-SF, Lab-sphere, Inc., North Sutton, NH). A beam size of 15 mm and port size of 45 mm was used. The optical properties were calculated from measured reflectance and transmittance with the inverse adding-doubling program.¹

3.2.1 India ink

We measured the absorption coefficients of the homogeneous and the aggregated India ink samples to be 0.3 mm^{-1} and 0.9 mm^{-1} respectively. With our 1.4 mm thick samples this meant that the transmittance of the homogeneous sample was 40 % less than the transmittance of the aggregated sample. If the samples had been 5 mm thick the transmittance of the aggregated sample would have been twenty times the transmittance of the homogeneous sample. These results show that in our case the absorption coefficient is no longer linearly dependent on the India ink concentration. The absorption coefficient of the all samples is presented in Figure 3. Another interesting discovery can also be seen in the figure, the absorption coefficient of the aggregated India ink sample completely lacks the normal wavelength dependency of the India ink. The aggregated India ink particles appear as black dots which completely block all wavelengths, thus making the spectrum flat.

The figure 4 shows the scattering coefficient of all the samples. For the homogeneous India ink sample the scattering was undetectable but for the aggregated sample an average scattering of 0.015 mm^{-1} was measured over the wavelength range of 350 - 850 nm. The increased scattering is due to the increased particle size in aggregated sample.

3.2.2 TiO_2

The aggregation changes the reduced scattering coefficient of the TiO_2 samples from 1.2 mm^{-1} to 0.9 mm^{-1} at 633 nm. The less significant difference compared to the aggregation in India ink samples is likely caused by weaker aggregation but unfortunately we were unable to characterize the rate of aggregation. As expected the aggregation of the TiO_2 does not change the absorption coefficient of the samples from zero. The absorption at the lower end of spectrum is due to the polyurethane.

4. CONCLUSION

In this paper we presented how the homogeneity of the sample affects the optical properties significantly. The increased aggregation decreases both absorption coefficient and scattering coefficient. It also breaks the linear relationship between the concentration of additive and optical coefficient. We see this phenomenon as a powerful tool in making more realistic calibration standards. It can also help to understand the inhomogeneities of the real measurement targets.

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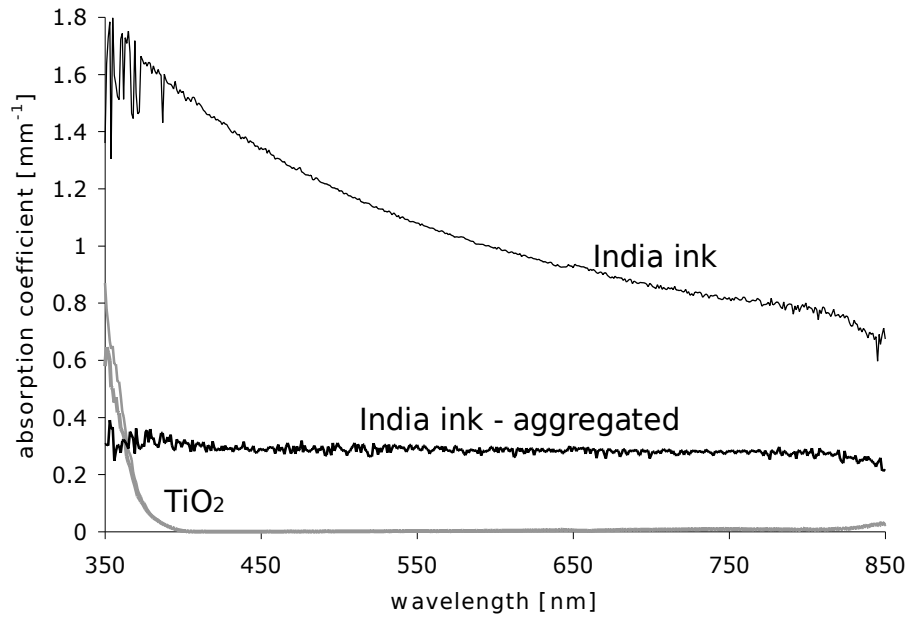


Figure 3. Absorption coefficient of the samples

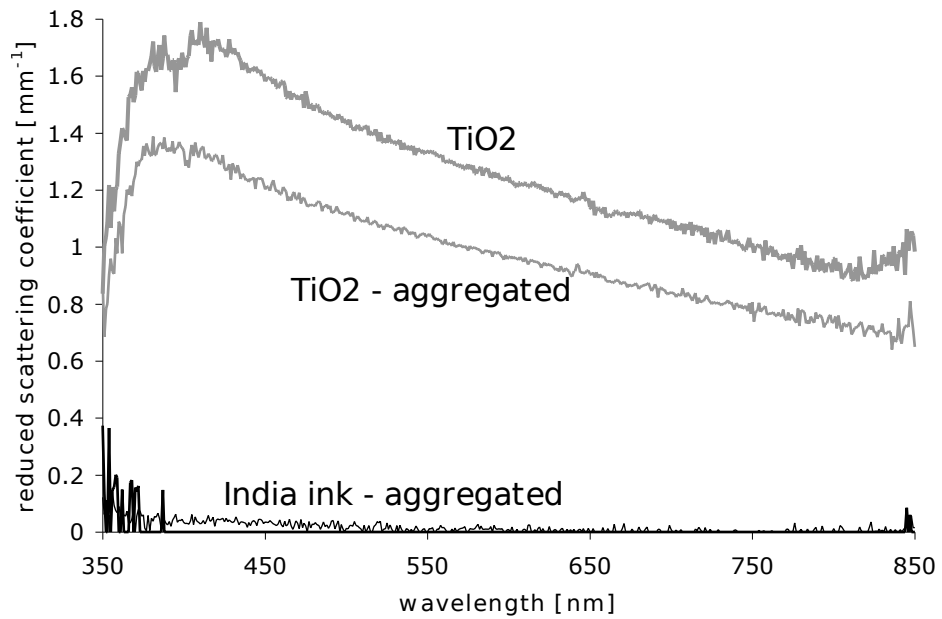


Figure 4. Scattering coefficient of the samples

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- [1] Moffitt, T., Chen, Y.-C., and Prahl, S. A., "Preparation and characterization of polyurethane optical phantoms," *Journal of Biomedical Optics* 11(4), 041103 (2006).