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Editorial

Special Issue on Diffuse Optical Spectroscopy: Advances towards Widespread Applications

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1. Introduction

Light is a powerful tool for the non-invasive and non-destructive analysis of several organic and inorganic materials. In particular, light scattering samples can be probed with different techniques depending on the required penetration. Though diffuse reflectance spectroscopy/near-infrared spectroscopy is typically focused on the outer regions of the sample under investigation [1–4], diffuse correlation spectroscopy, diffuse optical imaging/tomography, and functional near-infrared spectroscopy target a depth of few centimeters from the sample surface [5–8].

These techniques have already demonstrated their applicability in a number of interesting scenarios, such as the analysis of human tissues, food, wood, and pharmaceuticals. However, their full potential is yet to be unleashed, possibly leading to their future widespread use outside research laboratories, from large clinical installations down to consumer appliances. Indeed, in the years to come, it might be possible to use normal smartphones to verify the ripening of a fruit before picking it from the tree or buying it or to complement our traditional domestic diagnostic medical device kits with a cerebral/muscle oximeter. The main requirement for this purpose is to develop novel strategies to master the complexity of the physics/physiology (e.g., knowledge of the absorption spectra of basic constituents, modeling of heterogeneities, management of the interplay between measurables and measurement conditions, and probe contact artifacts). Moreover, to maximize performance and reduce costs, there is still the need for impressive technological progress. Finally, to solidly ground new developments and realizations, it is mandatory to enforce performance assessment and standardization strategies. Accordingly, this Special Issue has the ambitious aim to make further steps in these directions.

2. Contributions in the Special Issue

The paper by G. Qiu et al. [9] contributes to knowledge of the applicability of Fourier transform near-infrared (FT-NIR) spectroscopy. Because established techniques for cultivar analysis are destructive, expensive, and slow, the authors of this paper propose a combination of FT-NIR spectroscopy and discriminant analysis for the cultivar classification of sweet corn seeds. Their method was tested on 760 seed samples and allowed them to obtain a high classification accuracy (>99%), thus demonstrating the feasibility of the approach.

The work by S. Bock et al. [10] deals with the characterization of pure dielectric micro/nano powders with diffuse reflectance spectroscopy (DRS). Their methodology for preparing suitable samples of powder pellets in a well-reproducible way and granting high-quality DRS data/analysis is meticulously detailed, like a user manual, enabling laymen to approach this field for the first time.

The study by J.D. Veesa and H. Dehghani [11] proposes an approach to improve the accuracy of continuous-wave near-infrared spectroscopy (CW-NIRS) measurements of layered structures such as the human head that was devised to overcome the non-uniqueness of the solution of the diffusion equation by exploiting information derived from multiple measurement points and multiple wavelengths. In this way, in silico, both the tissue oxygenation index and the top layer thickness were recovered with an error of ≤4.4% in bilayer structures. An in vivo feasibility test was also reported and complemented the work.

In the same field, G. Maira et al. [12] reported the design, characterization, and validation of the tissue-mimicking phantom of a CW-NIRS device for brain functional imaging. Their prototype consisted of 12 dual-wavelength laser sources and 13 silicon photomultiplier (SiPM) detectors arranged inside an 8×8 cm^2 area. The main advantage of their architecture is the absence of optical fibers (which are typical sources of losses and artefacts) and the use of SiPMs (offering high signal-to-noise ratios).

In the field of diffuse correlation spectroscopy (DCS), K. Vishwanath and S. Zanfardino [13] applied an established theoretical model to analyze unconventional short source–detector separation measurements, which are unavoidable when analyzing small samples (e.g., small animals) or in constrained scenarios (e.g., endoscopy). With both in silico and on tissue mimicking phantoms, the authors demonstrated that the model could work well not only at traditional source–detector distances but also down to 1.5 mm.

The paper by S. Vasudevan et al. [14] presents a multimodal approach that combines few-wavelength frequency-domain (FD) NIRS and broadband CW-NIRS acquisitions. It is capable of drastically increasing the quantification accuracy of tumor-like perturbations in diffuse optical imaging scenarios down to a depth of 1 cm, mainly targeting breast cancer diagnosis.

In their work, E. Hernandez-Martin and J.L. Gonzalez-Mora [15] propose the use of an analysis algorithm based on Bayesian filtering for the CW diffuse optical tomography (DOT) of the human brain. Their approach was shown to be more robust and reliable in the reduction of background physiological noise (due to, e.g., heart rate or ventilation) during in vivo measurements.

Y. Lai et al. [16] present a functional near-infrared spectroscopy (fNIRS) study performed on 20 children with a commercially available CW device. Their goal was to quantify the effect on the updating function of the working memory of coordinative exercise interventions. The authors detected improved performance in the experimental group with respect to the control one in combination with evidence of a larger blood oxygenation increase during the task in the prefrontal area.

The paper by Ferocino et al. [17] presents the development of a time-domain (TD) DOT simulation platform used to estimate the in silico performance of a hand-held probe also under development in their research group. They demonstrated a significant improvement in the quantification of the perturbation absorption coefficient (<10% error) down to a depth of 2 cm.

The work by S. Konugolu Venkata Sekar et al. [18] is a comprehensive review of the latest advances in the field of broadband TD diffuse optical spectroscopy (DOS), dealing with its history, physical concepts, key instruments in the world, main analysis methods, possible applications, standardization of performance assessment procedures, and future outlook for the field.

The work by A. Dalla Mora et al. [19] overviews 15 years of research in the field of time-gated photon detection applied to TD-DOS. This paper covers its key physical concepts, main technologies for its implementation, most important open challenges, and possible applications.

3. Conclusions

This Special Issue reports advances in different light-based investigation techniques applied to scattering media. The path towards the exploitation of the full potential of scattered light remains long, but ongoing research is progressively overcoming different bottlenecks to achieve the final goal of widespread adoption.

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References

1. Kortüm, G. *Reflectance Spectroscopy: Principles, Methods, Applications*; Springer: Berlin/Heidelberg, Germany, 1969.
2. Germer, T.A.; Zwinkels, J.C.; Tsai, B.K. *Spectrophotometry: Accurate Measurement of Optical Properties of Materials*; Elsevier: Amsterdam, The Netherlands, 2014.
3. Griffiths, P.R.; De Haseth, J.A. *Fourier Transform Infrared Spectrometry*, 2nd ed.; Wiley: Hoboken, NJ, USA, 2007.
4. Movasaghi, Z.; Rehman, S.; ur Rehman, I. Fourier Transform Infrared (FTIR) Spectroscopy of Biological Tissues. *Appl. Spectrosc. Rev.* **2008**, *43*, 134–179. [CrossRef]
5. Durduran, T.; Choe, R.; Baker, W.B.; Yodh, A.G. Diffuse optics for tissue monitoring and tomography. *Rep. Prog. Phys.* **2010**, *73*, 076701. [CrossRef] [PubMed]
6. Yodh, A.; Chance, B. Spectroscopy and imaging with diffusing light. *Phys. Today* **1995**, *48*, 34–40. [CrossRef]
7. Martelli, F.; Del Bianco, S.; Ismaelli, A.; Zaccanti, G. *Light Propagation through Biological Tissue*; SPIE: Bellingham, WA, USA, 2010.
8. Pifferi, A.; Contini, D.; Dalla Mora, A.; Farina, A.; Spinelli, L.; Torricelli, A. New frontiers in time-domain diffuse optics, a review. *J. Biomed. Opt.* **2016**, *21*, 046011. [CrossRef] [PubMed]
9. Qiu, G.; Lü, E.; Wang, N.; Lu, H.; Wang, F.; Zeng, F. Cultivar Classification of Single Sweet Corn Seed Using Fourier Transform Near-Infrared Spectroscopy Combined with Discriminant Analysis. *Appl. Sci.* **2019**, *9*, 1530. [CrossRef]
10. Bock, S.; Kijatkin, C.; Berben, D.; Imlau, M. Absorption and Remission Characterization of Pure, Dielectric (Nano-)Powders Using Diffuse Reflectance Spectroscopy: An End-To-End Instruction. *Appl. Sci.* **2019**, *9*, 4933. [CrossRef]
11. Veesa, J.D.; Dehghani, H. Hyper-spectral Recovery of Cerebral and Extra-Cerebral Tissue Properties Using Continuous Wave Near-Infrared Spectroscopic Data. *Appl. Sci.* **2019**, *9*, 2836. [CrossRef]
12. Maira, G.; Chiarelli, A.M.; Brafa, S.; Libertino, S.; Fallica, G.; Merla, A.; Lombardo, S. Imaging System Based on Silicon Photomultipliers and Light Emitting Diodes for Functional Near-Infrared Spectroscopy. *Appl. Sci.* **2020**, *10*, 1068. [CrossRef]
13. Vishwanath, K.; Zanfardino, S. Diffuse Correlation Spectroscopy at Short Source-Detector Separations: Simulations, Experiments and Theoretical Modeling. *Appl. Sci.* **2019**, *9*, 3047. [CrossRef]
14. Vasudevan, S.; Forghani, F.; Campbell, C.; Bedford, S.; O'Sullivan, T.D. Method for Quantitative Broadband Diffuse Optical Spectroscopy of Tumor-Like Inclusions. *Appl. Sci.* **2020**, *10*, 1419. [CrossRef]
15. Hernandez-Martin, E.; Gonzalez-Mora, J.L. Diffuse Optical Tomography Using Bayesian Filtering in the Human Brain. *Appl. Sci.* **2020**, *10*, 3399. [CrossRef]
16. Lai, Y.; Wang, Z.; Yue, G.H.; Jiang, C. Determining Whether Tennis Benefits the Updating Function in Young Children: A Functional Near-Infrared Spectroscopy Study. *Appl. Sci.* **2020**, *10*, 407. [CrossRef]
17. Ferocino, E.; Pifferi, A.; Arridge, S.; Martelli, F.; Taroni, P.; Farina, A. Multi Simulation Platform for Time Domain Diffuse Optical Tomography: An Application to a Compact Hand-Held Reflectance Probe. *Appl. Sci.* **2019**, *9*, 2849. [CrossRef]
18. Konugolu Venkata Sekar, S.; Lanka, P.; Farina, A.; Dalla Mora, A.; Andersson-Engels, S.; Taroni, P.; Pifferi, A. Broadband Time Domain Diffuse Optical Reflectance Spectroscopy: A Review of Systems, Methods, and Applications. *Appl. Sci.* **2019**, *9*, 5465. [CrossRef]
19. Dalla Mora, A.; Di Sieno, L.; Re, R.; Pifferi, A.; Contini, D. Time-Gated Single-Photon Detection in Time-Domain Diffuse Optics: A Review. *Appl. Sci.* **2020**, *10*, 1101. [CrossRef]