

REVIEW



Advances in Optical Analysis of Materials and Complex Biological Systems Using Infrared Spectroscopy

Andrew J. Macnab^{1, 2,*}

¹University of British Columbia, Canada

²Stellenbosch Institute for Advanced Study, Wallenberg Research Centre, South Africa

Abstract: Infrared spectroscopy (IRS) is an increasingly important optical technique because the properties of light in this part of the electromagnetic spectrum enable interactions with materials and complex biological systems that provide unique information that has both research and commercial applications. This review summarizes the basic optical principles employed in IRS systems and outlines recent technological advances that have improved the functionality and applicability of IRS instruments. The relevance of the principal practical applications of near-infrared spectroscopy (NIRS), mid-infrared spectroscopy (MIRS), and hyperspectral imaging (HI) in materials science, agriculture, and medicine is highlighted, and key progress made with the software used for the analysis of raw optical data is described. The shorter wavelengths in the near-infrared (NIR) range of the spectrum achieve greater penetration than those in the mid-NIR range. NIRS is now a prominent analytical technology, and its growing role in medicine is the principal focus of this review. MIRS is an important and widely used sample characterization and analytical technique. NIR HI enables the chemical constituents in a sample to be analyzed by capturing complete spectral data at each sample point; the unique spectral signatures generated then allow different chemicals to be visualized and identified.

Keywords: chromophore, biomedical optics, light-emitting diodes, spatially resolved geometry, spectra

1. Infrared Spectroscopy

Infrared spectroscopy (IRS) is an optical technique used to analyze the interaction between infrared (IR) radiation and matter [1]. Conventionally, while IRS utilizes wavelengths between 800 and 12500 nanometers (nm), the IR portion of the electromagnetic spectrum is divided into near-, mid-, and far-IR regions named for their relation to the visible spectrum [2]. IR spectrometers measure the absorption by, emission from and/or transmission through a macroscopic sample; the spectra generated are analyzed graphically, with IR absorbance plotted against frequency or wavelength [3]. IRS techniques allow the identification and characterization of chemical substances in solid, liquid, or gaseous forms, and are now a widely used method for analysis and measurement.

Because the shorter wavelengths in the near-IR (NIR) range achieve greater penetration than those in the mid-NIR range, near-infrared spectroscopy (NIRS) can monitor physiological change in a wide range of biological materials [1, 4]; the prominent role of NIRS in medicine is the principal focus of this review. Mid-infrared spectroscopy (MIRS) is a widely used sample characterization and analytical technique, and NIR hyperspectral

imaging (HI) enables the chemical constituents in a sample to be analyzed by capturing complete spectral data at each sample point [1, 2].

The existence of an IR element beyond the visible spectrum of light was first identified by Herschel in 1800 when he was working with sunlight. Having detected that there was a temperature gradient between the red and violet ends of the spectrum, he then measured the temperature beyond the visible red portion and found it to be the highest of all. A series of advances over the next two centuries has increased our understanding of what were termed “caloric or invisible rays” at the time and are now known as IR light and the electromagnetic spectrum. Discoveries made related to the IR portion have led to technological applications that have relevance today for both scientific research and industrial purposes (Table 1).

2. Near-Infrared Spectroscopy

The properties of the far-, mid-, and near-IR regions of the electromagnetic spectrum are shown in Table 2. NIRS uses light in the NIR region of the electromagnetic spectrum, spanning wavelengths from 780 to 2500 nm. For applications involving the interrogation of biological tissues, the wavelength range usually extends from 760 to 1000 nm, as this is where the wavelengths with peak absorption for the chromophores of interest are found. These are nominally

*Corresponding author: Andrew J. Macnab, University of British Columbia, Canada and Stellenbosch Institute for Advanced Study, Wallenberg Research Centre, South Africa. Email: andrew.macnab@ubc.ca

Table 1
Timeline highlighting IRS milestones and their relevance, from Herchel’s initial discovery to its current status as a key analytical tool for science and industry

Year	Discovery	Relevance
1800	Herschel discovered infrared radiation	The temperature gradient between the red and violet ends of the spectrum in sunlight and significant heating beyond red light defines the infrared region
1881	Abney and Festing pioneered IR studies of molecular structure	This allowed the absorption spectra of multiple organic liquids to be identified
1889	Ångström recorded molecular vibrational frequencies	This establishes that IR absorption originates from molecular not atomic vibrations
Early 1900s	Extensive research by Coblenz led to the first IR spectrometer	This work established the unique IR spectra for specific compounds
1957	Perkin-Elmer developed the first low-cost infrared spectrometer	This instrument made practical spectroscopy a reality
1960s	Norris developed the first near-infrared (NIR) spectrometer	This enabled the production of quality NIR spectrometers
1970	Fourier-transform infrared spectroscopy developed	Acquisition of high-resolution spectral data improves measurement accuracy
1977	Jobsis reported that brain tissue can be interrogated within the NIR range	The first real-time, noninvasive studies of brain blood volume and oxygenation follow
2000s	Development of the first hyperspectral imaging instruments	Studies in space conducted; rapid adoption for agriculture and environmental monitoring
Present day	Continuous technological evolution, expansion of analysis methodology, miniaturization of devices and lower cost	Wide use of IRS for commercial applications and scientific research is now possible

Table 2
Properties of the far-, mid-, and near-infrared regions of the electromagnetic spectrum

Microwave	Far-IR	Mid-IR	Near-IR	Visible light
Wavelength	1000–25 μm	25–2.5 μm	2.5–0.75 μm	
Wavenumber	33 cm ⁻¹	330 cm ⁻¹	3300 cm ⁻¹	12800 cm ⁻¹
Frequency	1.0 × 10 ¹² Hz	1.0 × 10 ¹³ Hz	1.0 × 10 ¹⁴ Hz	3.8 × 10 ¹⁴ Hz
Energy	6.6 × 10 ⁻²² J	6.6 × 10 ⁻²¹ J	6.6 × 10 ⁻²⁰ J	2.5 × 10 ⁻¹⁹ J

850 nm for oxyhemoglobin (O₂Hb), 760 nm for deoxygenated hemoglobin (HHb), and 975 nm for water (H₂O) [4–6].

2.1. Advantages of NIRS for material analysis

NIR photons have many advantages as an energy source; principally because NIRS employs non-ionizing radiation and is noninvasive, little or no sample preparation is required, no chemicals are used, and in most applications the technique is rapid, accurate, nondestructive, and inexpensive. NIRS is not only broadly applied to monitor physiological change in human tissue but is also widely used to define the properties of new materials and as the method of choice for analysis and quality control in multiple fields. The most prominent commercial applications relate to agriculture; others include analysis of food, meat, fish, milk, fruit and vegetables, wine, beer, wood, soil, petrochemicals, cosmetics, and pharmaceuticals [1, 2].

2.2. Principal uses of NIRS

1) Agriculture

NIRS was first used to measure the protein and moisture content of wheat, and the data obtained are still the basis of

trading standards. NIRS can accurately measure the chemical composition of wheat; however, another parameter of commercial value is analysis of nutritive values, and research indicates that IRS-derived methodologies are potentially better in this regard than assessment of chemical composition or reliance on agronomic characteristics [7].

2) Materials science

Techniques have been developed for quality control of a range of foods, chemicals, textiles, and biological compounds. For example, the film thickness of microscopic samples can be measured, and the characteristics of nanoparticles and optical coatings can be identified.

3) Biomedical science

Two unique features make NIR light energy invaluable for studying human physiology: (1) the ability of NIR photons to pass through the skin and penetrate subcutaneous tissue and (2) the wavelength-specific peak absorption characteristics of two chromophores of interest, O₂Hb and HHb [4, 6]. NIRS instruments that incorporate two different wavelengths (usually 760 and 850 nm) enable changes in concentration from the baseline of each chromophore to be monitored in real time and the total

hemoglobin in the tissue sample to be derived ($O_2Hb + HHb$) as a measure of blood volume. In this way, NIRS provides a means of monitoring change in both tissue oxygenation and hemodynamics [5, 6].

As with all forms of IRS, because NIRS is an optical technology, accurate measurement when instruments are used transcutaneously is dependent on transmission of sufficient photons through the skin into the tissue of interest; it is also a requisite that as much light energy as possible returning from the interrogated tissue is also captured. Hence, ideally, both skin tone and subcutaneous adipose tissue thickness are accounted for in order to achieve optimal accuracy [8]. However, from a practical standpoint, with instruments that use the 760 and 850 nm wavelengths, only minimal signal attenuation is usually encountered even in pigmented subjects, which means that physiological changes of interest can readily be observed [9]. While this includes trends involving the hemodynamic effects of neuroexcitation in the cortex during cerebral monitoring, skin pigmentation has been shown to affect the accuracy of absolute measures of cerebral regional oxygen saturation (rSo₂), although the magnitude of this effect appears to depend on the specific NIRS platform used [10].

2.3. Advances in NIRS technology

The broad range of applications for which NIRS can now be used has evolved due to advances across several aspects of the technology. This has involved the evolution of NIRS instruments through the use of new materials and design innovations. In particular, the availability of light-emitting diodes (LEDs) as a light source negates the necessity to use the lasers employed in the earliest iterations of NIR spectroscopy [5]. Also, LEDs are inexpensive and can be driven with low power, making spectrometers possible that are small in size, complexity, and cost, so miniature devices are now constructed as self-contained entities incorporating NIR light emission and photodetection, with a rechargeable power supply and wireless capability [11].

Improvements in basic algorithms for data capture, the availability of increasingly refined software for conversion of raw optical data to graphic outputs, and multivariate analysis have raised the acceptability of NIRS systems in terms of accuracy and “user friendliness.” Lower costs have made devices more accessible for commercial and laboratory use as well as for scientific study and patient monitoring in medicine.

As in all forms of IR spectroscopy, ongoing collaboration between scientists from different disciplines remains central to defining and overcoming the limitations inherent in NIRS applications and to improving the capabilities and relevance of the technique for the analysis of new materials and in medicine.

2.4. Human physiology driving applications of NIRS

The most extensive body of research employing NIRS relates to studies of muscle physiology. In addition to the changes from baseline in oxy, deoxy, and total hemoglobin concentration generated in muscle in response to hypoxia and ischemia, a large number of absolute measures reflecting physiological effects related to hemodynamic and oxygenation changes that quantify muscle fitness have been validated [6].

Applications of NIRS specific to medicine have also evolved due to a greater understanding of human physiology; in addition, challenges faced in clinical care, laboratory studies, and improvements in IRS technology have contributed. Premature newborns are an example of where the physiological characteristics of

specific human populations influence the medical care they require, and much research has explored monitoring technologies with the potential to improve care [12].

A premature newborn has an immature neurovascular supply. The duplication of vessels in the brain needed to ensure the supply of blood to key areas is not as fully developed as it is in an infant born at full term. Similarly, a premature infant's ability to autoregulate blood flow to the brain to maintain oxygen delivery during fluctuations in systemic blood flow is also not fully developed. Hence, these infants are at risk of brain damage due to inadequate provision of oxygen, which makes the ability to measure brain oxygen parameters central to their care [13].

Problematically, early techniques were complex as they involved percutaneous aspiration of arterial blood from the radial artery or later depended on catheterization of the umbilical arteries, which can only be used for the first few days of life.

The evolution of oximetry improved this situation to a significant degree, and early technology was akin to spectroscopy in that it used light energy from the red zone of the electromagnetic spectrum to monitor the “redness” of oxyhemoglobin in tissue as a measure of the level of oxygen being carried by red cells. Significantly, it was only with the development of data analysis software that converted optical data into a numerical value displayed as a percentage that the use of oximetry became feasible at the bedside and, hence, relevant in a clinical context [14]. There are parallels with how the relevance of IRS monitoring modalities and their clinical adoption have benefited from improvements in data processing methodology and the development of diagnostic algorithms able to match data to reference spectra in real time.

Although a major step forward, the practicality of oximetric measurement of peripheral oxygenation was limited because the availability of oxygen is obviously physiologically most critical in the brain. Consequently, more than 50 years ago, initial trials were conducted using NIRS to monitor oxygenation and hemodynamic parameters in the brain in premature babies, but challenges were soon identified, which required improvements in the hardware and software before valid measurements relevant to their care became feasible [12].

Then, over the last decade, the rapid expansion of research trialing prototype IRS devices able to monitor cerebral oxygenation occurred [15]. Early evidence indicated the potential for NIRS-guided brain protection strategies to improve neurologic outcome after complex cardiac surgery; this led to further device refinement, followed by clinical trials of devices able to monitor changes in cerebral oxygenation that are now able to contribute to critical care-related decision-making [16].

Two other physiological challenges that have driven IRS research are (1) how to avoid ischemic injury to the spinal cord during surgery involving the aorta and (2) how to optimize neurologic recovery following acute traumatic spinal cord injury [17, 18].

Experimentation has led to the development of several intra-operative adjuncts that are considered effective in spinal cord protection during vascular surgery; the most promising methods involve derivatives of transcutaneous and invasive NIRS technologies that are able to quantify regional tissue oxygenation [18].

After traumatic spinal cord injury, maintenance of mean arterial pressure (MAP) to optimize cord perfusion and oxygen delivery is a complex yet critical factor related to functional recovery. Hence, invasive monitoring has been trialed in animal models using miniature multiwavelength NIR sensors designed to be implanted surgically over the dura of the injured cord. The aim ultimately is to provide clinicians with real-time hemodynamic and oxygenation data able to add the precision required to support MAP optimally in injured humans [17].

2.5. Future directions

Practical applications using NIRS systems will increase exponentially. In medicine, this will be especially true for brain functional NIRS (fNIRS), as this application of spectroscopy is becoming a viable alternative to functional magnetic resonance imaging (fMRI), which, while still the “gold standard,” is not readily available in practice due to cost, complexity, and limited hardware. NIRS will also become a key component of multimodal neuromonitoring in neonatal intensive care during treatment with neuroprotective strategies and will contribute to identifying new therapies for babies at risk for brain damage [19].

fNIRS is recognized as a particularly practical alternative to magnetic resonance imaging (MRI) due to its low cost and portability; however, its lower spatial resolution is a limiting factor. But, as with other IR spectroscopic techniques, ongoing advances in hardware will likely lead to a growing number of practical applications for fNIRS, as will software advances that improve the accuracy of data preprocessing. fNIRS promises to expand our insights into brain connectivity and provide a new understanding of mechanistic factors related to disease.

It is now evident that fNIRS of the brain combined with simultaneous transcutaneous bladder NIRS can provide unique physiological information that is not available to clinicians by other means; in the future, such combined studies will likely yield information relevant to an enhanced ability to evaluate the mechanisms associated with bladder disease, identify new approaches to therapy, and assess the effects of treatment [12, 20].

Wearable devices able to continuously monitor physiological variables will become mainstream and increasingly relevant for disease prevention, personalized medicine, real-time health monitoring, and home-based serial data collection [21, 22]. Because of the continued development of electronics, biocompatible materials, and nanomaterials, these wearable devices will be available in differing forms, such as accessories, integrated clothing, and body implants.

3. Mid-Infrared Spectroscopy

Mid-infrared (MIR) spectroscopy measures the absorption of IR light in the MIR range (2,500–25,000 nanometers) and is used to analyze the molecular composition of substances. The resulting spectrum is a measured response (reflectance, absorbance, conductivity) as a function of some systemic portion of a continuum (wavelength, frequency). The organic material and mineral components in the sample affect the MIR spectrum [1, 2]. MIR photons interact with both organic and inorganic molecules to provide inherent molecular sensitivity [23].

As MIRS technology has advanced, its flexibility and broad applicability have revolutionized multiple applications in diverse fields; these are becoming increasingly varied in nature, ranging from agriculture and the food sector, through to materials science, industry, and environmental studies. A particularly important recent advance has been the development of advanced spectral acquisition techniques, and this, in addition to the innovative use of materials for generating, guiding, and detecting MIR radiation, has enabled MIRS to evolve into a state-of-the-art tool [24].

3.1. Advantages and limitations of MIRS for materials analysis

The primary advantages of MIRS are the speed and reliability of the technique compared to other analytical methods,

the fact that it is nondestructive and can provide simultaneous qualitative and quantitative characterization of a wide variety of samples and that it is suited to the analysis of sensitive materials [25, 26].

Limitations include the potential for water vapor to interfere with the analysis of samples and the complex preparation required to make some materials suitable for analysis. Also, not all substances have characteristic IR absorption bands and so do not lend themselves to IRS, and complex mixtures can generate signals that are difficult to interpret due to overlapping spectral peaks [25].

3.2. Principal uses of MIRS

MIR spectroscopy is widely used in fields such as chemistry, pharmaceutical science, and environmental analysis for identifying materials and monitoring chemical processes by providing detailed information about molecular structure and composition.

Samples can be in gas, liquid, or solid form. MIRS is extensively used for applications requiring qualitative analysis and provides either functional group or structural information about a sample, its composition, or a “fingerprint” spectrum for identification of a material [26].

1) Soil analysis

This application provides fast estimates of soil properties for classification and monitoring of composition, texture, and mineralogy. Soil analysis using reflectance spectroscopy can employ visible, NIR, and MIR wavelengths. Representative literature describes the most suitable spectral regions for specific soils, reviews the soil properties that can be predicted and their level of accuracy, and compares in-field versus laboratory spectral techniques [27, 28].

Decreasing spectrometer costs and developments in IRS and related software algorithms have increased the use of IRS for soil analysis. Techniques allow rapid acquisition of soil information for use in agriculture and environmental monitoring and can provide results comparable in accuracy to many traditional extractive and digestion laboratory methods. Examples include the estimation of lime requirement, organic carbon content, and levels of exchangeable cations, air-dry moisture, clay content, and biological indicators [28].

2) Environmental monitoring

MIRS techniques aid environmental analysis including the detection of pollutants and the monitoring of greenhouse gases.

In low- and middle-income countries in particular, science-based approaches employing MIRS are relied on to monitor the environment and accelerate agricultural development. MIRS now plays a key role in providing a workable surveillance framework because the technology can provide rapid, low-cost, and highly reproducible diagnostic screening [29].

3) Chemical and pharmaceutical industries

Here, MIRS is used for quality control and to confirm the identity of raw materials and the active compounds present in drugs.

The fast and nondestructive nature of mid-NIR analytical techniques can provide chemical and physical information of virtually any matrix. Combining these analytical techniques with multivariate data analysis makes many forms of qualitative and quantitative measurements possible that are relevant to

pharmaceutical product analysis and quality control. Literature reviews the range of NIR applications applicable to the pharmaceutical industry, techniques for raw material identification and qualification, and methods for direct analysis of intact solid tablet forms [30].

4) Food, wine, and beer

The concentration of compounds in food products and alcoholic beverages is measured using MIRS techniques, and the detection of impurities and foreign compounds provides quality assurance and avoidance of contamination [31].

For example, measurement of the concentration of the widely consumed stimulant caffeine is a legislated requirement, and the study of caffeine continues to be the focus of a range of research projects because of its relevance to, and impact on, human health. Globally, the food, wine, and beer industries are also required to be compliant with multiple national and international regulations, which require constituent analysis and quality control of the majority of their products, hence the importance of reliable, commercially cost-effective analytical methods and the proven benefits of MIRS-related techniques [32].

3.3. Future directions

Developments in solid-state physics, photonics, electronics, materials science, engineering, and informatics will lead to the next generation of IR light sources, signal transducers, and detectors. Such advancements in mid-IR spectroscopy will enable more refined, task-specific tuning of device performance and advance the sensitivity and precision of measurement [33].

4. Hyperspectral Imaging

The combination of NIRS with digital imaging provides HI. The HI technique obtains a spectrum for each pixel in the image to identify materials, detect objects, or detect processes, and can describe the distribution of constituents within a sample [1, 34].

HI sensors collect a series of images over a narrow wavelength range across the electromagnetic spectrum, which are combined to form a three-dimensional hyperspectral data cube for analysis.

4.1. Advantages and constraints of hyperspectral imaging

HI systems have the ability to look at objects using a wide portion of the electromagnetic spectrum. Particular objects leave a unique spectral “fingerprint,” and modern sensor technology makes it possible for HI to cover large sections of the earth’s surface with exceptional spatial, spectral, and temporal resolution [34]. The “fingerprints” generated are known as spectral signatures, and these enable the identification of the materials that make up the scanned object. For example, a spectral signature for oil helps geologists find new oil reserves and aids in the detection and clean-up of oil spills. It is the ability to extract a desired spectral signature from high-dimensional remotely sensed hyperspectral imagery that allows objects to be detected and identified over large geographic areas.

Constraints limiting wider adoption of HI include the high cost of equipment and the need for technical expertise to operate HI systems and interpret the data generated. The volume of data acquired is high because of the technique’s extensive spectral coverage; this necessitates both large storage capacity and experience using the complex analytic algorithms. HI is also unsuited to some

applications due to its lower spatial resolution compared to other imaging methods and where environmental conditions adversely impact data quality. In addition, the current lack of universal standards negatively impacts data sharing and compatibility between different systems.

4.2. Principal uses of HI

The ability of HI to identify various minerals makes it ideal for geology and mining, where the technique can be used to rapidly identify minerals that have commercial interest. Its use has also spread into fields as diverse as astronomy, agriculture, molecular biology, biomedical imaging, physics, military security, and surveillance [35].

HI instruments can be mounted on drones and used for military surveillance; hyperspectral thermal IR emission measurements detect differences in the relative radiance spectra from various targets. The technology is also employed in systems used for facial recognition [36].

Widely used in agriculture, HI enables the health of crops to be monitored. In addition, the quality and safety of agricultural and food products can be assessed; for example, by screening for contamination by foreign proteins in animal feed to prevent the transmission of bovine spongiform encephalopathy (mad cow disease).

4.3. Advances in HI data processing

Open-source deep learning models can now be used to enhance NIR HI data processing. An example is the challenge presented to fruit importers of how to acquire quality data parameters where their product is tightly packed in boxes; this can be overcome by using models from the computer vision domain [37]. These new AI approaches can provide viable solutions in situations like this, where, in contrast, conventional HI data analysis using traditional techniques would be problematic.

4.4. Future directions

HI will benefit particularly from advances in machine learning and future increases in computing capacity. Integration of deep learning models to automate feature extraction will aid analysis-based decision-making [38]. Further miniaturization of components is expected to improve real-time applications by making lighter-weight, more portable systems available for use in locations remote from the laboratory. Advances related to real-time image processing will also increase efficiency in the field and particularly advance the capability of technology used for surveillance and environmental monitoring.

The strengths, limitations, and applicability of near-, mid-, and far-IR spectroscopy are summarized in Table 3.

5. The Evolution of Spectroscopic Applications in Medicine

Ways in which IRS technologies have been refined within the field of medicine provide an example of how progressive evolution can adapt and refine spectrometers, data collection, and analytic methods to more effectively meet the requirements of specific end-users.

In medicine, applications that use spectroscopy come about because of a combination of clinical need and innovative advances in technology, such as happened with the advent of magnetic

Table 3
Strengths, limitations, and applicability of near-, mid-, and far-IR spectroscopy

	Near-Infrared	Mid-Infrared	Far-Infrared
Strengths	Photon penetration into tissue Wavelength-dependent chromophore absorption Noninvasive Non-ionizing radiation Portable Chemical free Nondestructive Relatively low cost	Biomolecule analysis Provides absorption bands for complex molecules Molecular structure and composition of samples High sensitivity/selectivity Nondestructive Low sample requirements Versatile applications Suited to quality control	Facilitates visualization of the distribution of different chemical components within a sample Collects a spectrum at each pixel of the image Samples can be in solid, liquid, or gaseous forms Characterization of new materials
Limitations	Lower sensitivity than MIRS Effectiveness limited by sample thickness Complex samples require preprocessing Photon attenuation by fat and pigmented skin	Sensitivity to water vapor compromises measurement Some samples require complex preparation Less effective for materials without strong MIR absorption characteristics Overlapping spectral peaks	Expensive technology Requires expert operators Data storage needs are high, and analysis is complex Environmental conditions impact analytic potential Limited spatial resolution No universal standards
Applicability	Primarily used for real-time monitoring of tissue oxygenation and perfusion and analysis of overtone/combinations of molecular vibrations Multiple commercial applications Method of choice for quality control	Primarily used for chemical and biological detection and to identify unique molecular fingerprints The detailed chemical signatures obtained are widely used by industry, in agriculture, and for gas sensing and environmental monitoring of pollutants	Primarily used for chemical and biological detection, environmental monitoring, and chemical detection. Ideal for analyzing complex mixtures like polymers and gases due to its ability to identify unique molecular fingerprints

resonance spectroscopy (MRS) [39]. The ability to combine MRS with MRI has led to magnetic resonance spectroscopic imaging, which is able to provide both spatial images of anatomic structure and spectroscopic data that allows visualization of metabolic activity within the body.

As emphasized previously, clinician scientists must understand the physiology underlying the clinical issue for which they are seeking to apply a technology such as spectroscopy and, equally importantly, must be fully aware of exactly what a new technology can and cannot do. Full comprehension of both elements is essential; otherwise, questions will be asked of the technology that cannot be answered, and the potential value of an otherwise promising and valid technique risks being misunderstood and incorrectly dismissed, as happened in early NIRS studies in urology [40].

What Pasteur said is also relevant: “In the fields of observation chance only favours the prepared mind.” In other words, happenstance will only result in progress if those involved have the ability to see the relevance of an otherwise seemingly arbitrary observation, or of a finding that at first glance seems inconsistent or incorrect. An example of how the latter scenario applies to IRS is the situation that led to the discovery that NIRS could be applied to study the bladder in health and disease [5].

5.1. The evolution of NIRS applications in urologic science

In a piglet model, an NIRS emitter-detector array was placed on the lower abdomen in a study looking for spectroscopic changes in the brain; the lower abdominal channel was intended to

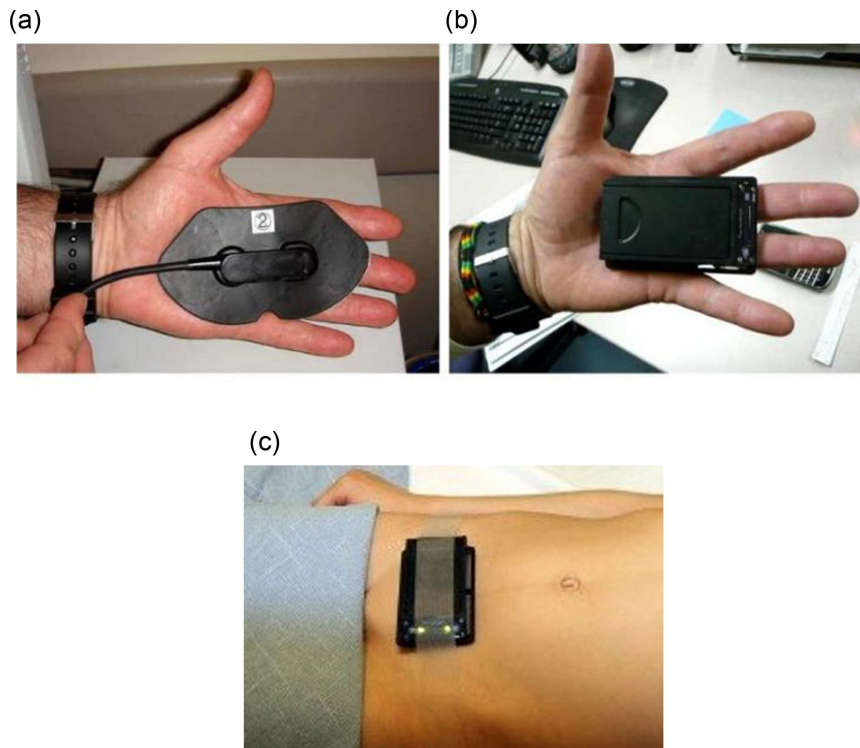
provide control data against which the anticipated changes in the brain could be compared. However, the abdominal sensor detected fluctuations in chromophore concentration at regular intervals. While these were initially considered to represent “electromagnetic interference” or “random noise,” careful review identified that the changes were reproducible, and ultimately, it was recognized that they coincided with when the animal’s bladder became full, and voiding then followed. Changes in bladder hemodynamics and oxygen supply during urine storage and emptying had not been identified previously. A subsequent human study confirmed the ability of transcutaneous NIRS to interrogate the anterior wall of the bladder [5].

Over time, the first generation of bench-top laser-powered spectrometers that required a large light-occluding patient interface containing the optical emitter-detector array were superseded by small, self-contained, wireless devices with light-emitting diodes as the light source (Figure 1). These devices made it possible to transcutaneously monitor the anterior wall of the bladder in ambulant patients. Subsequent studies by multiple independent investigators indicated that changes in chromophore concentration occurring in the bladder detrusor muscle during voiding differed between health and disease [21]. Moreover, noninvasive NIRS of the bladder proved to be equally discriminant for the diagnosis of bladder outlet obstruction as the invasive “gold standard” test of urodynamic pressure flow studies (UDS) in men with prostatic disease [5, 9, 21].

The relevance of this application of IRS is emphasized by the global impact that hypertrophy of the prostate gland causes on the quality of life of the majority of men as they age. Lower urinary tract symptoms occur with increasing frequency due to progressive bladder outlet obstruction; the urgency and nocturia that result affect both morbidity and quality of life.

Figure 1

The progressive miniaturization possible with the availability of light-emitting diodes (LEDs). (a) The patient interface from a bench-top laser-powered spectrometer that required a fiberoptic cable to link the spectrometer to the patient, (b) a miniature wearable instrument with LEDs as the light source, and (c) a fully self-contained wireless near-infrared spectrometer positioned on the lower abdomen of a child to transcutaneously monitor her bladder



Problematically, the test conventionally used to diagnose the condition is invasive; investigation using UDS requires urethral and rectal catheterization; most men find these invasive elements unpleasant, and consequently, many who need the test decline to be studied. Also, there is a significant complication rate with infection following catheterization, so this test can only be repeated at intervals [9]. In contrast, NIRS of the bladder is noninvasive, patient friendly, and safer than catheterization as it requires only that the patient spontaneously void with a small device taped to the skin over the bladder, and so can be repeated as often as needed [5, 9, 20].

The initial proof of principle validating NIRS against urodynamic pressure flow studies included the construct of a regression tree algorithm [5]. Nowadays, integration of machine learning techniques and deep learning algorithms is a promising approach to improving accuracy and precision of NIRS systems; a particular strength is the ability of deep learning models to enhance sensor-based bladder monitoring by automatically identifying suitable representations from raw input data [41].

Recent reviews underscore the importance of this bladder monitoring application of IRS as a way to improve the well-being of those with several forms of bladder dysfunction and advance the management of urinary incontinence [9, 20, 21]. Also, NIRS systems that capture bladder and brain data simultaneously can now define new physiological dimensions, which make a more comprehensive evaluation of bladder control and voiding function possible [9].

Consequently, optical diagnostics are seen to have the potential to transform bladder assessment and redefine precision medicine in urology, and ultimately, NIRS-based monitoring will

likely be used to improve patient outcomes and quality of life through a home-based model of bladder care [9].

5.2. NIRS monitoring of the brain and spinal cord pathways

Adequate brain oxygenation is a fundamental physiological requirement, hence the relevance of modern methodologies for directly monitoring this element of brain function using NIRS [42]. The systems now available to monitor the brain and spinal cord (described in Section 2.4) are examples of where specific refinements were needed before spectroscopy could effectively meet what was required clinically. The miniaturization and improvements to the sensors incorporated now enable them to monitor changes in cortical oxygenation transcutaneously. In addition, the components of the sensor incorporate the spatially resolved geometry of the emitter-detector array and transmit NIR photons in reflectance mode. These features, coupled with sophisticated software, make real-time trend monitoring of the regional tissue oxygen saturation of hemoglobin (rStO₂) in the brain possible.

Cerebral rStO₂ provides real-time, end-organ information on perfusion-oxygenation, and research is beginning to identify how these systems can be used to drive care-related interventions that will potentially improve the clinical management of premature babies [16, 19]. Similar technology that provides NIRS-derived brain oxygenation parameters is used to improve patient monitoring during anesthesia and in critical care units [13, 16].

Neuroscience relies increasingly on fMRI. However, the cost and limitations of fMRI are making fNIRS an increasingly

attractive alternative. As technical reviews outline, the advantages of fNIRS include systems that are portable, easy to apply, generally tolerant to body movement, can be combined with other modalities such as electrophysiology, and are suited to use across patient populations from the newborn to the elderly [43, 44]. Recent literature also identifies fNIRS as a valuable tool in neurodegenerative diseases and confirms its potential to analyze multiple elements of brain function [45].

fNIRS has matured into an especially versatile tool in cognitive developmental neuroscience, where the advantages of the technology become particularly apparent when studying infants and young children who suffer from neurological, behavioral, and cognitive impairment [44]. However, spontaneous activity in small infants does make their data vulnerable to noise from motion artifacts, hence the benefit of recent advances in data preprocessing using accurate channel pruning.

The advantages of fNIRS over fMRI are also exemplified by its growing use in neuroscience applications related to the integrity of functional pathways in the brain and spinal cord, for example, those integral to continence. The existence and importance of these pathways were demonstrated initially using fMRI, but studies directly comparing the two modalities have confirmed the validity of fNIRS in this context [46].

Similar dynamic changes in blood oxygenation in the bilateral frontal cortex were detected using fNIRS as were identified using fMRI and positron emission tomography, and the increased levels of cortical oxyhemoglobin detected became stronger as the bladder reached capacity [47].

This is relevant, as problematically, the use of fMRI is not feasible in everyday clinical practice for urologists wanting to study the “brain bladder continuum” as a causal mechanism for lower urinary tract symptoms. However, as evaluation of the brain-mediated mechanisms involved using fNIRS is now feasible, this provides an important alternative to fMRI [35], and research is providing a growing body of evidence documenting how the storage of urine, sensation when the bladder is full, and control of bladder emptying all depend on an extensive network of pathways and interconnected brain regions [48].

Simultaneous NIRS measurements of the bladder and fNIRS of the frontal brain cortex can now be conducted during bladder filling; the fNIRS system used has multiple emitter-detector arrays integrated into a head cap that provide 23-channel monitoring [20]. This system can detect the increase in cortical oxyhemoglobin concentration that occurs in the frontal cortex associated with awareness of a sensation of urgency and the need to void; this neuroexcitation precedes triggering of the pontine micturition pathway that then initiates bladder emptying. Significantly, fNIRS has identified that this cortical neuroexcitation and associated urgency to void can be ablated by a distractor stimulus; this offers the potential for future research to identify forms of behavioral modification that are effective in controlling urge incontinence.

5.3. NIRS applications in women’s health

Pelvic floor muscle (PFM) dysfunction due to childbirth and/or the effects of aging negatively impacts the health and quality of life of millions of women worldwide, due to associated forms of urinary incontinence. Kegel exercises, which can help to strengthen the muscles of the pelvic floor that control the flow of urine, are the cornerstone of remedial care [20]. However, no objective measures exist that allow PFM strength or fitness to be quantified; this is a challenge for clinicians and a motivational

problem for women who are unable to know if their remedial Kegel exercise regimen is generating benefit.

A novel transvaginal interface that incorporates NIR emitter-detector arrays now allows NIRS-derived measurement of the physiological effects of sustained maximal contraction of the PFM in women [5, 49]. From these data, a validated parameter used to evaluate muscle fitness in athletes has been translated to quantify PFM fitness as a baseline diagnostic measure for clinicians and as a means of quantifying the effects of remedial therapy for women. In this parameter, the half recovery time for reoxygenation is calculated from the slope of recovery of oxygenation following a sustained maximal voluntary contraction of the PFM; the more rapidly reoxygenation occurs, the better the PFM is meeting the metabolic demands of muscular work [5].

6. IRS Integration in Personal Monitoring Devices

Tele-diagnostics is a burgeoning area with high potential for IR-based tools [50]. The popularity of wearable monitoring systems made possible by the technical breakthroughs that have led to miniature wearable and smartphone-linked sensors has created a huge commercial market. Many of these devices incorporate IR technologies, which enable critical biomarkers to be continuously measured. In addition to providing the wearer with personal health data in real time, today’s wearable devices also offer a significant opportunity for the advancement of tele-diagnostics and home-based data collection. When linked to software on smartphones some can already be used to detect cardiac functional and structural pathology, and by saving results remotely, the comprehensive serial data obtained can then be shared with physicians to enhance their diagnostic capability [22].

7. Conclusion

IRS is an optical technique of increasing importance because the properties of light in this part of the electromagnetic spectrum enable interactions with materials and complex biological systems that provide unique information. IRS has become an invaluable tool in the context of research and a range of industrial applications, many of which have an important commercial role. The ability to identify and characterize molecules is central to the relevance of this technology, and ongoing refinement of devices and advances in data capture and analysis continue to increase the applicability of IRS. The ability to provide unique spectral fingerprints now makes this technology an essential element in the high standards currently achieved in fields as diverse as environmental monitoring, pharmaceutical analysis, food safety, pollutant detection, polymer science, semiconductor manufacturing, and clinical monitoring and diagnostics. And, as further advances can be expected in near-, mid-, and far-IRS technologies, this field is one on which an increasing number of research scientists will come to rely for optical analysis of materials and complex biological systems.

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Ethical Statement

This study does not contain any studies with human or animal subjects performed by the author.

Conflicts of Interest

The author declares that he has no conflicts of interest to this work.

Data Availability Statement

Data sharing is not applicable to this article as no new data were created or analyzed in this study.

Author Contribution Statement

Andrew J. Macnab: Conceptualization, Methodology, Validation, Formal analysis, Investigation, Resources, Data curation, Writing – original draft, Writing – review & editing, Visualization, Project administration.

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