JPhys Photonics

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To cite this article: Lien Smeesters *et al* 2025 *J. Phys. Photonics* **7** 032501

IOP Publishing J. Phys. Photonics 7 (2025) 032501 https://doi.org/10.1088/2515-7647/adbea9

Journal of Physics: Photonics

CrossMark

OPEN ACCESS

RECEIVED
23 May 2024

REVISED
15 January 2025

ACCEPTED FOR PUBLICATION
10 March 2025

PUBLISHED
19 June 2025

ROADMAP

2025 photonics for agrifood roadmap: towards a sustainable and healthier planet

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Keywords: agriculture, spectroscopy, photonics, agrifood industry, optical sensors, machine learning, AI

Abstract

Photonics technologies play a crucial role in driving technological advancements within the agrifood industry, aiming to deliver a sustainable food and agriculture, and offering healthy, nutritious and safe food for all of us. Particularly, optical sensors and imaging systems, together with machine-learning processing and advanced lighting, play a pivotal role in monitoring crop and soil health with unprecedented precision, while safeguarding the food supply chain. This roadmap aims to provide an overview of the state-of-the-art photonics technologies benefitting agrifood applications, including a view on their current limitations, challenges and future potential, while addressing practical case studies. Future trends towards multimodal sensors and sensor fusion, artificial intelligence and digital twins, miniaturization and controlled farming are highlighted. The revolutionizing capabilities of the photonics technologies are indicated, inspiring future applications and developments, and paving the way towards optimized resource utilization, increased crop yields, stopping land degradation and reduction of food waste.

Contents

1. Introduction

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The agrifood industry has been subject to strong digitalization and technological advances during the last decades, including the introduction of Internet of Things (IoT), smart machinery, machine vision inspection systems, and the introduction of precision farming [1, 2]. However, continuous technological developments remain indispensable to tackle the current and future challenges, aiming to deliver a sustainable food and agriculture production, and to offer healthy, nutritious and safe food for all of us. Key challenges include population growth, food waste, food and feed quality, global warming, stopping land degradation and minimizing the use of resources and pesticides. The world population is expected to grow to 10 billion people by 2050, as estimated by the Food and Agriculture Organization (FAO), requiring a dramatic food and feed production increase of 60% [3]. On the other hand, one third of all food produced is currently wasted during production, processing, distribution or at the consumer [4]. In addition, food scandals linked to safety and traceability have been marking headlines for centuries, impacting consumer trust, as reported by the EIT Food Trust Report indicating a consumer confidence of only 55% regarding product safety and 43% for product authenticity [5]. Different food contaminants still sneak into the food chain, among others, pesticide residues, pathogenic microorganisms, and mycotoxins [6]. Food fraud, including mislabeling, dilution, and adulteration is still affecting a wide range of products, among others, olive oil, milk, seafood, coffee and sugar [7]. Finally, in view of mitigating climate change, a transition to sustainable agriculture is indispensable, since agrifood accounts for 70% of the global water use and 24% of the greenhouse gas emissions [8], while climate change is envisioned to strongly challenge the agrifood industry increasing the presence of toxins and affecting the soil and harvest quality.

Photonics technologies play a crucial role in tackling these challenges, by the development of novel optical sensors, imaging systems, smart labels, and lighting [9, 10]. As main advantages, optical spectroscopic sensors and imaging systems offer a non-destructive and chemical-free evaluation, suitable for both individual spot checks and in-line autonomous monitoring. In general, photonics technologies have the potential to impact the whole food supply chain (figure 1), revolutionizing the industry [1, 2]. On the field, drones and agricultural machines (e.g. tractors, plucking robots) supplemented with multi-/hyper-spectral imaging technologies are being deployed for irrigation, fertilizer monitoring, pest and diseases detection. Visible cameras feature shape inspection, and the detection of foreign objects and anomalies, while near-infrared spectroscopy (NIRS) enables measuring nutrients, proteins and sugars. Soil evaluation benefits from distributed fiber Bragg detectors, which offer root and moisture monitoring capabilities. Light detection and ranging (Lidar) is a valuable technology for the mapping of plants. Fluorescence spectroscopy is useful to monitor toxins, amino acids, vitamins, allergens, and pigments, while Raman spectroscopy (RS) enables determining biochemical components like sugars, lipids, water, and proteins. Terahertz spectroscopy is employed, among others, to monitor the leaf moisture content. Handheld and smartphone-connected spectrometers are entering the food chain, with the potential for deployment along the whole supply chain. The global market for photonics for precision agriculture (PA) is currently worth around 4.6 billion euros and is expected to virtually double by 2027 to a value of 9.1 billion euros, corresponding to an annual growth of around 15% [2].

Future trends

Continued monitoring and digitalization of the entire food chain, from farm to fork, is indispensable to enhance sustainability, both environmentally and socially, while offering full transparency and traceability. Photonics technology advances are further required to enable a broader deployment, addressing the cost, size, efficiency and sensitivity, while also considering sample handling, technology useability, robustness, system calibration, seasonal and biological variation. In addition, these technologies are also envisioned to contribute to the EU Soil Deal aiming to manage and safeguard soils for future generations [11], as well as to

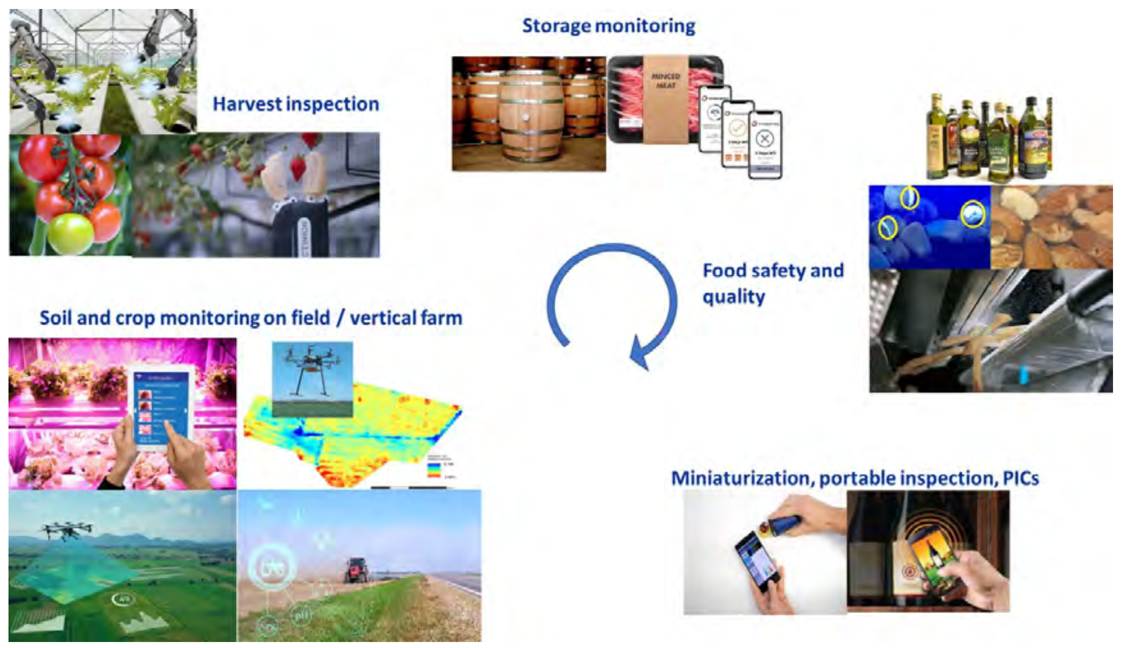

Figure 1. Photonics technologies benefitting the full agrifood supply chain.

the Farm to Fork Strategy that is defined within the European Green Deal and aims for sustainable, environmental-friendly food systems [12], and to the United Nations Sustainable Development Goals, and in particularly Goal 2 on Zero Hunger.

Driven by the novel developments, the following key trends can be identified:

1. Multimodal sensors combining different sensing technologies within a single unit or device. Combining multiple optical sensor technologies enables to extend the sensing capabilities, enabling multi-element detection, while offering an improved sensitivity and accuracy [10]. For example, combination of absorption and light scattering can provide both insight into the starch and moisture content while also giving insights in the firmness of the product, and combination of absorption and fluorescence spectroscopy might enable a multi-mycotoxin sensing covering both fluorescent and non-fluorescent toxins. In addition, sensor fusion can be exploited to improve the calibration, standardization, and robustness of the current sensors.
2. Miniaturization towards handheld devices and photonic integrated circuits (PICs) [13]. The availability of miniaturized and handheld spectrometer units has been empowering mobile spectroscopy [2]. PICs are driving further miniaturization, offering the potential of adding highly precise sensing functionalities on single low-power and miniaturized chips, giving rise to a cost-effective and scalable technology.
3. Advanced data processing based on machine learning (ML) and artificial intelligence (AI), benefitting the sensitivity and selectivity within predictive, prescriptive and adaptive processes within the whole food supply chain, including soil monitoring, weed management, disease detection, product sorting and food water management [14–16]. The generation of adequate and complete training sets is of indispensable importance to ensure a robust model, while the processing and sensing technologies are ideally being optimized in synergy. Digital twins (DTs), in combination with AI, might enable the generation of digital plants and animals, helping the prediction algorithm.
4. Sensor-data fusion and enhanced interoperability of data. Future efforts should be made towards the standardization of photonics data, and a network for data transfer and fusion is requested to ensure its implementation in smart agriculture.
5. Indoor, controlled farming, including vertical urban farming, driven by new sensor and lighting technologies. The controlled environment enables continuous monitoring of the plant's health, maximizing yield and reducing economic losses. State-of-the-art sensing technologies, making use of hyperspectral imaging (HSI), have indicated a $100\times$ higher crop yield than traditional farming, and using 98% less soil and 95% less water [17], while offering the potential to measure macro-elements such as nitrogen, phosphorus, and potassium. Specialized energy-efficient LED and lighting algorithms can furthermore optimize growth and yield. Additionally, a trend towards the application of quantum dots

(QD) for spectroscopy and vertical farming can be observed, optimizing e.g. the sunlight spectrum in greenhouses and contributing to a more efficient light use [18, 19].

6. The journey of space exploration is expected to expand significantly in the near future. This expansion carries the potential to reshape our understanding of the cosmos while offering tangible benefits for life on our home planet. Challenges arise in meeting the nutritional needs of astronauts and future space colonists in the extreme space conditions, given the objectives of returning humans to the Moon, the long-term exploration of Mars, the growth of space tourism, and the continued operation of the International Space Station. The roadmap outlined here shows photonic technologies as highly suitable for various space food applications. Examples include the use of UV lighting for plant growth systems in space, as well as for water purification. Also, spectroscopic and imaging techniques are instrumental for identifying contaminants and monitoring nutritional content, and sensors are essential to detect spoilage or degradation of food products during storage [20].

Photonics for agriculture and food processing is today still emerging, but represents a fast-growing segment with a compound annual growth rate (CAGR) of 14% [20]. Lighting and UV disinfection are dominant segments, since lighting advancements enhance growth in greenhouses and vertical farms, and UV is crucial for e.g. irrigation and plant immunity. Second, imaging systems are of major importance, which can be used on drones and agriculture robots. Hyper—and multi-spectral imaging systems have been increasingly implemented, as well as thermal camera systems. We expect this will be further boosted by emerging imaging technologies, including polarization multispectral imaging, x-ray imaging, and THz imaging [21]. Additionally, we believe the miniaturization of the spectroscopic sensing technologies towards handheld and pocket-size devices has a huge potential that will revolutionize the agriculture and food industry in the coming years. In general, an increased use of photonics technologies along the full supply chain is envisioned, where photonics sensors are implemented in a wide range of devices and infrastructures, such as tractors, drones, robotic arms and mobile robotic modules, machine vision and inspection systems, and storage and transport. The increased availability of real-time and continuous monitoring tools will benefit an improved food quality and safety for all of us.

Roadmap objectives

The roadmap aims to provide an overview of the state-of-the-art photonics technologies benefitting agrifood applications, including a view of their current challenges and future potential. Chapter 1 discusses image-based monitoring and ML processing, while chapter 2 focuses on spectrometry and spectral sensors. Chapter 3 gives a view of the miniaturization of optical sensors, including handheld devices and PICs. Chapter 4 discusses lighting and light source optimization, both for indoor farming and spectroscopy applications. Each chapter includes both general contributions that provide a general overview of the technology, and case-studies that illustrate the technology for a certain challenge within the agrifood industry. Finally, concluding remarks summarize the key messages of this roadmap.

Chapter 1: Image-based monitoring and machine learning

2. Automated routines based on optical sensors and ground-based or airborne robots for monitoring crop plants in experimental trials and agricultural fields—what are the needed framework conditions

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Status

With the rise of digital plant phenotyping [22, 23] the use of sensors to measure plant traits in greenhouse screening and experimental field sites has become state of the art. By this, the situation of plants in a specific environment can be assessed and described using explainable parameters in high throughput, objectively and reproducibly. By using machine or deep learning approaches, relevant parameters, such as the reaction to a specific stress can be evaluated qualitatively and quantitatively [24].

Commonly used sensor technologies range from simple RGB sensors to more complex multispectral, hyperspectral, thermal sensors or 3D technologies [25]. For all digital phenotyping technologies, data quality and compromise between spatial and spectral resolution are crucial. To bring sensors into the field, commonly they are mounted on uncrewed ground (UGV) or unmanned aerial vehicles (UAV). These vehicles usually are remotely controlled or follow a predefined route over the field. During the last few years, these systems have greatly improved in terms of the level of autonomous operation for data collection [26].

All these technologies assess an enormous amount of data and adequate technologies are required for interpretation and subsequent decision making. The analysis of the datasets is mainly performed by using state-of-the-art AI models that are based on huge human-annotated datasets [27] (see figure 2). A typical workflow therefore combines (i) implementation of a field experiment to acquire training data (ii) data acquisition (iii) data annotation by experts, (iv) training of the ML and deep learning models with feature importance reporting and finally (vi) explanation and result interpretation using agronomic knowledge [28]. With focus on plant pathology and assessment of plant diseases, significant steps have been made regarding fully automated counting of plants and plant coverage description [29], autonomous rating on single plant and on plot area [30] and integration of data acquisition, interpretation and decision making [31].

However, most of the methods developed from research did not made it beyond the proof-of-concept level and need intense reworking to enter a product level which can be used and integrated by practical farmers. Nevertheless, these developments are an impressive demonstration of what can be expected in the field of smart farming and PA. Future development will focus on sensor and analysis in a short term. Long term developments will target online processing of the data in the field as well as integration of these routines into practical agriculture.

Current and future challenges

A distinction is made between short-term and long-term approaches for plant phenotyping. Short-term means a period within five to ten years, while long-term describes a time horizon of more than ten years.

Imagine the scenario, that sensors are moved to and within the field by using unmanned vehicles like drones or robots. In recent years, huge effort has been made to increase the automation level of these vehicles in parallel with the car industry's motivation to produce autonomous cars. The big picture of an agricultural field managed by machines, autonomous flying drones [32] driving or walking robots [33] and the fully and integration of high resolution satellite data is hindered by incompatible regulations and laws as well as from unsolved problems in navigation and communication between actors on the field.

Today, researchers use different types of cameras, each camera type has different advantages and disadvantages. Complete camera-carrier systems are available as well as carriers with interchangeable sensors like RGB, multispectral or thermal cameras. Each system requires, in particular when multimodal data (data from different sources) is collected, internal and external calibration to provide proper and valid data that can be linked to further sensor data and provide georeferencing. While spectral signatures were used to recognize stress symptoms [34] the 3D geometry is described by stereo vision or 3D laser-scanners [35]. Each dataset is interpreted by sophisticated AI models. This adds semantics to the data and aims for the definition of a static or dynamic trait describing the plant status or behavior. AI means commonly deep learning approaches, which are much more difficult to explain, compared to traditional ML methods like SVM or Random Forest. However this explanation is needed when targeting or tailoring the hardware to the

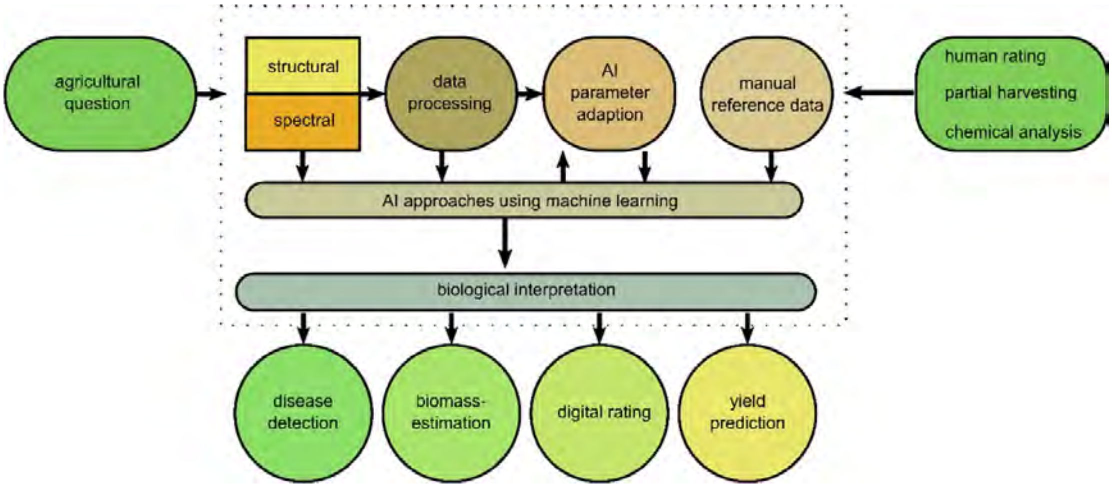

Figure 2. The workflow of an agricultural experiment. It includes the agricultural question, the data acquisition, the AI processing pipeline including the human expert's input and the target variables like disease or biomass estimation, digital rating or yield prediction.

application requirements. Finally, and besides all the complex research approaches, application within the field and in agricultural practice are demanded. A common example is the transfer from HSI in the greenhouse using hundreds of scanned channels to a cheaper and more robust multispectral open-field approach with five to six spectral channels [28]. If this transfer is successful, the next step of integrating the AI model into the sensor hardware, called edge AI can be tackled. Another aspect and challenge that needs to be addressed is the issue of data availability and data ownership. Current field experiments collect terabytes of data stored in 'closed silos' with metadata described in heterogeneous defined data formats. This makes it impossible to reuse or even to share the data within the community. Acknowledged standards are missing and we need approaches for data harmonization and sharing on an international level [36]). The current situation slows down transdisciplinary collaborations and the adaption of state-of-the-art algorithms to data of existing experiments.

Long-term challenges will need more time and attention as the user group is more heterogeneous. The biggest challenge is the integration of monitoring routines into practical agriculture as sensor based monitoring at different scales (ground (UGV), air (UAV) and orbit (satellites)), AI data analysis, strengthening the trust in AI solutions, defining evaluation routines for algorithms and standards, adapting rules and laws for the use of robots with a high degree of automation, improving the acceptance of digital methods and finally implementing digital flagship showcases with high radiance into the population (figure 3). Furthermore, the integration of multiple heterogeneous data collection stations for field parameters and microclimate into a (inter-) national forecast system for plant diseases and yield is required. This will lead to AI-supported decision-support systems for application recommendations and if used for an automated documentation system for agriculture. Finally, the main challenge will be to define management decisions and adopt daily routines based on the above-described automated approaches.

Advances in science and technology to meet challenges

UGV and UAV are dominant tools in plant science and are used especially on experimental field sites where the area is limited, and a high imaging resolution is required. However, their application in practical agriculture is so far very limited. Nevertheless, during the last years robots have been established especially for row crops with a high cost recovery contribution like sugar beet, salad, and vegetables. These robots are mainly used for weed control but integrate sensor racks and on-board analysis systems for a direct decision-making and application like the control of a spraying nozzle. The extension to other non-row crops, to other plant diseases or even the integration of modern field management strategies such as spot farming are possible [37].

All methods that use online processing on the field require a proper AI model that is capable to interpret the data. The ability to explain the model generally has become the gold standard for building trust and deployment of AI systems [38]. Thus, explainable AI (XAI) developed in recent years describes a suite of ML methods that enable humans to understand, trust and better explain models. Nevertheless, the model interpretability must be considered in combination with constraints and requirements like data- and model explainability, fairness and accountability.

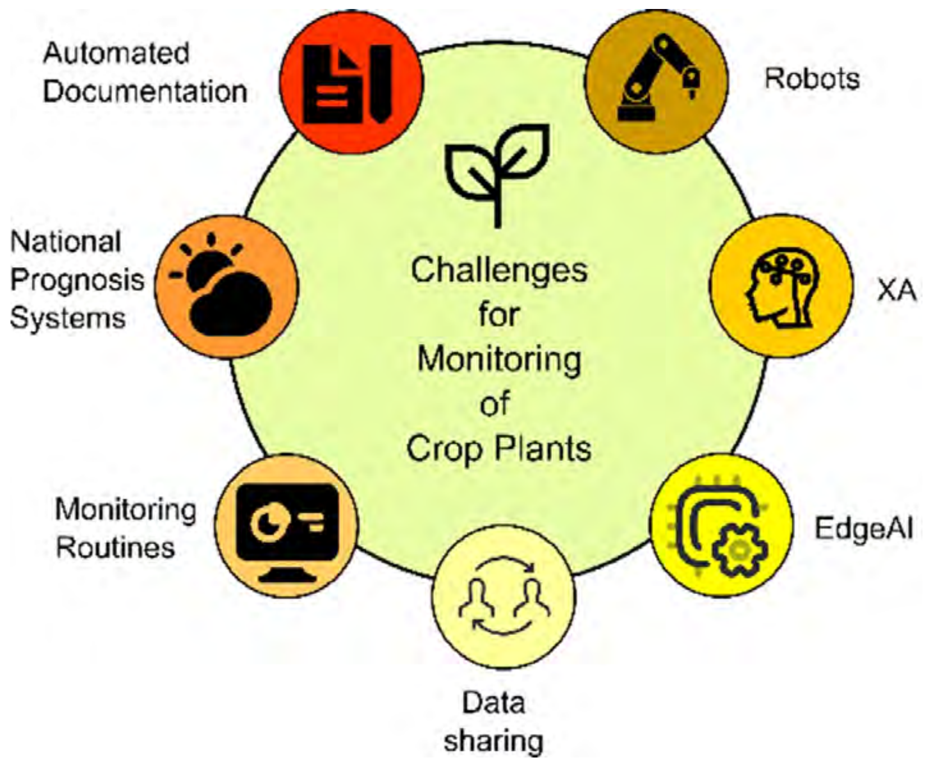

Figure 3. Challenges for monitoring crops in the field. While robots, explainable AI, edge AI and data sharing are short-term challenges, the integration of monitoring routines into practical agriculture, the implementation of national prognosis systems and the use of automated monitoring systems are depicted to be long-term goals.

As all AI methods rely on available data, data sharing is essential to encourage a multi-disciplinary cooperation. More and more funding organizations have integrated and made mandatory the FAIR principles (findability, accessibility, interoperability, and reusability) for data management [39]. In addition, the MIAPPE protocol has been published, an approach for Minimum Information About a Plant Phenotyping Experiment [40]. Although these tools exist, data sharing lacks problems like data misuse and missing harmonization, non-existing standards and the risk of eroding properties. Nevertheless, approaches based on blockchain ecosystems have been described in the literature, but a solid implementation is still missing [41].

Edge AI devices that integrate the model directly in the hardware just entered the market and enable the collection of semantic data instead of raw data. Providing sensors with a pre-trained model offers the chance to provide highly customized sensors tailored to the problem [42].

Nevertheless, most field experiments focus on a simple experimental setup to investigate methods for one specific factor or information of interest. We need more trials for data assessment in real world situations with mixed infections and combinations with abiotic stress like nutrient or water deficiencies, which increases the complexity of the problem. This complicates the transfer and integration of methods from research and experimental field sites into the demands of practical agriculture but is closer to the real situation.

Furthermore, local laws and regulations should make it possible to validate new applications and technologies in special test fields with limited scope, even beyond previously tested and permitted scenarios. This includes the utilization of larger payloads for research purposes, the use of innovative application technology, and deployment on prototype carrier platforms. This would decisively strengthen the innovative power and, above all, the contemporary adaptation of regulation.

A further aspect is the availability of climate data for the agricultural fields. In the case of plant diseases, for example, decision making can be supported by a proper microclimate forecast of temperature and humidity of adjacent weather stations. By integration of small microclimate stations distributed across the country and provided vendor-independent by companies and individuals, this disease forecast can be fundamentally enhanced in its quality by a national prognosis system. This also requires, an improved infrastructure and availability of specific technologies in rural areas.

Finally, monitoring and an automated decision-support system can help to automate the farmers documentation obligations. This requires a harmonized field and farm management system similar to ISO-bus which controls the devices of a tractor.

Concluding remarks

This summary shows potential technical fields where a disruptive change in the way sensors, data and analysis models will be used in future can be expected. It has been shown, that either prototypes or at least concepts for the changes have been published or currently entered the marked.

Monitoring crop plants in the field is today a multidisciplinary approach covering technicians, farmers, AI-specialists, and engineers. The shown approaches for data sharing highlighted have perhaps the greatest impact, as data availability will encourage researchers worldwide to work on problems with existing data. The limitation here is not technical, but more a motivation problem. Data harmonization and the definition of obligatory standards is the first step to not just combine different disciplines in a team, but to motivate groups of different disciplines to work together internationally.

This, together with the expected development of new technologies such as sensor fusion, Edge AI, and robots will transform agriculture (see figure 3). Here, the idea of PA, doing the right at the right place at the right time, will be leading for all applications.

Acknowledgments

This study was partially funded by the Deutsche Forschungsgemeinschaft (DFG; German Research Foundation) under Germany's Excellence Strategy—EXC 2070-390732324.

In addition the study is partially funded by the German Federal Ministry of Food and Agriculture (BMEL) on the basis of a resolution of the German Bundestag. The project is sponsored by the Federal Agency for Agriculture and Food (Bundesanstalt für Landwirtschaft und Ernährung, BLE) within the framework of the digitization strategy of the BMEL, call funding code 28DE104A18.

3. Thermal IR imaging in agriculture. Recent advancements and future trends

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Status

Thermal IR imaging encompasses the collection, analysis, and interpretation of data predominantly obtained within the thermal infrared IR portion of the electromagnetic spectrum, and it could be employed in agriculture both on the field or in a remote sensing configuration. IR remote sensing commonly acknowledged in vegetation research spans from 3 to 14 μm, which is further categorized into the mid-wave infrared (MWIR) range of 3–5 μm and the long-wave infrared (LWIR) range of 8–14 μm. The MWIR sensor detects radiation that is emitted by the Earth as well as radiation that is reflected from the Sun. On the other hand, the LWIR sensor is primarily influenced by the emitted radiation [43]. Extensive research has been conducted on the remote sensing of vegetation in the visible and near-infrared (VNIR) range (0.3–1.0 μm) and shortwave infrared (SWIR) range (1.0–2.5 μm), with a specific focus on the analysis of biochemical and biophysical properties of vegetation [44]. Nevertheless, the spectral data obtained from the VNIR and SWIR domains are insufficient in capturing the complete range of structural and chemical attributes exhibited by plants. To face this issue, hyperspectral and multispectral imaging can be employed. Specifically, HSI provides a detailed spectral analysis across a wide range of wavelengths, enabling the detection of specific biochemical properties of plants [45], whereas multispectral imaging, while less detailed than HSI, strikes a balance by providing sufficient information for various agricultural assessments without the complexity of hyperspectral data, which requires complicated processing for its interpretation [45]. Notably, it should be highlighted that the key absorption qualities of specific vegetative components, such as polysaccharides (e.g. cellulose) and leaf surface attributes (e.g. waxes and hairs), are situated in the thermal infrared domain [46]. The advancement of technology in the field of thermal IR spectrometers and sensors has facilitated the increase in the utilization of thermal IR imaging in the agricultural sector in recent years [47]. This can be attributed to the decreased costs of the equipment and the straightforward operational procedures, which have opened up possibilities for its implementation in various areas of the agricultural and food industries. Furthermore, efforts are currently being made to enhance its compatibility with precision farming practices [48]. The thermal characteristics of plant leaves are influenced by a multifaceted and heterogeneous interior structure, which encompasses a specific quantity of water per unit area. Therefore, the potential for conducting research on individual plants using thermal remote sensing is feasible due to the versatile, accurate, and high-resolution capabilities of infrared thermography [47]. However, the precision of thermal measurements is contingent upon the prevailing environmental circumstances, as these factors have a direct impact on the thermal characteristics of the observed crop. Hence, it is imperative to calibrate pictures based on meteorological conditions in order to facilitate the comparison of image data acquired throughout distinct measurement intervals and growth seasons. Therefore, calibration of images according to weather conditions is necessary for comparison between image data obtained during different measuring periods and growth seasons [47]. Moreover, in order to compare images, the soil water content (SWC) should be estimated [49]. In this perspective, an effective approach based on the use of multivariate statistical analysis, such as partial least squares (PLSs) regression, has been proposed for adjusting thermal measurements based on environmental variables [50]. This technique allows for the development of models that can predict thermal responses under varying conditions, thus enhancing the reliability of thermal imaging in agricultural applications. Thermal remote sensing technology has the potential to be applied across various agricultural materials and processes, encompassing situations where heat is either generated or lost throughout spatial and temporal dimensions [51]. The potential application of thermography in the field of agriculture encompasses various areas such as monitoring nurseries, scheduling irrigation and harvesting, detecting, identifying diseases and pathogens, crop health monitoring, evaluating ripeness, and detecting bruises, as reported in figure 4.

Current and future challenges

Thermal IR technology has proven very beneficial in PA due to its ability to non-invasively and efficiently monitor and assess many aspects of crop health and environmental conditions. Specifically, thermal IR imaging allows academics and practitioners to get valuable information about how plants react to stress, improve the way resources are managed, and increase agricultural production. Research has highlighted the significance of thermal imaging in studying the relationship between plants and their environment, making

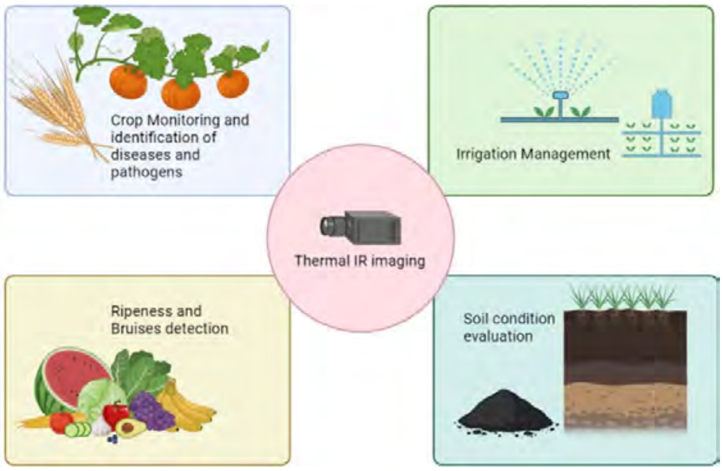

Figure 4. Examples of the most spread applications of thermal IR imaging in agriculture. This technology could help in crop monitoring, ripeness and bruises detection, soil conditions evaluation and irrigation management. This figure is created in Biorender.com.

it a widely used technology in the fields of agronomy and environmental sciences [52]. In addition, thermal IR imaging is widely recognized as an essential technique in PA for monitoring crop health, identifying stress, and analyzing the environment [53]. Concerning the evaluation of plant stress, thermal IR imaging has played a crucial role in evaluating plant stress in several scenarios, including those with high salt levels and water scarcity in rice farming [54] and citrus trees in greenhouses [55], showing its ability to evaluate the water condition of plants. Particularly, thermal IR imaging is able to assess plant stress responses by tracking fluctuations in leaf temperature, which indicate changes in plant physiology under different stress scenarios. Research has shown the efficacy of thermal imaging in identifying plant distress caused by reduced rates of photosynthesis and transpiration or scarce water condition [52, 56]. Particularly, thermal imaging allows for the real-time evaluation of plant responses to stress factors such as drought by monitoring leaf temperature and angle, which serve as early-stage markers of plant stress [57, 58]. Importantly, the surface temperature of plants is regarded as a highly responsive indication of stress, frequently anticipating the manifestation of apparent symptoms [59]. By integrating thermal imaging with multispectral imaging, researchers may get a holistic comprehension of the physiological reactions of plants under stress [60].

It is worth to highlight that thermal IR imaging was used to evaluate not only the temperature of the leaves, but also of the soil. Particularly, thermal imaging may be used to evaluate SWC and its distribution, and this technology provides extensive insights for this purpose. For instance, Tian *et al* developed a thermo-time domain reflectometry (T-TDR) probe capable of monitoring the water content and thermal characteristics of unfrozen soil, as well as measuring the amount of ice in partly frozen soils [61]. Similarly, Qiu & Zhao devised an algorithm using thermal imaging and the three-temperatures model (3 T model) to gauge soil evaporation and soil water status [62]. This technique showcases the capacity of thermal imaging to track the movement of water in soil and the pace at which it evaporates.

Thermal IR imaging has emerged as a helpful technique in assessing seeds in nurseries because of its non-destructive characteristics and capacity to provide important information on seed quality and viability. Research has shown that thermal imaging may be used to observe several factors associated with the health and quality of seeds. These factors include seed viability, the health of transplants, the quality of graft unions, and the identification of physiological diseases [52, 63]. Moreover, thermal imaging methods have been used to diagnose seed viability without causing harm during the process of seed absorption, through image processing and statistical algorithms [64]. This demonstrates the efficiency of thermal imaging in evaluating the health of seeds under controlled environmental settings [65, 66]. To examine the disparities between the coldest and hottest seedlings using thermal imaging, it is essential to take into account the thermal reactions of the seedlings under different environmental circumstances. Prior research has emphasized the importance of thermal imaging in observing how plants react to fluctuations in temperature and stressors, demonstrating its capability to assess identify physiological processes such the closing of stomata and water deficiency stress [67, 68]. Regarding seedlings, the thermal response refers to the impact of temperature on the growth and development of plants. Studies have shown that exposing seedlings to warm temperature conditions during their first development stage might affect their ability to withstand stressors such as oxidative stress and transpirational water usage in the future [69].

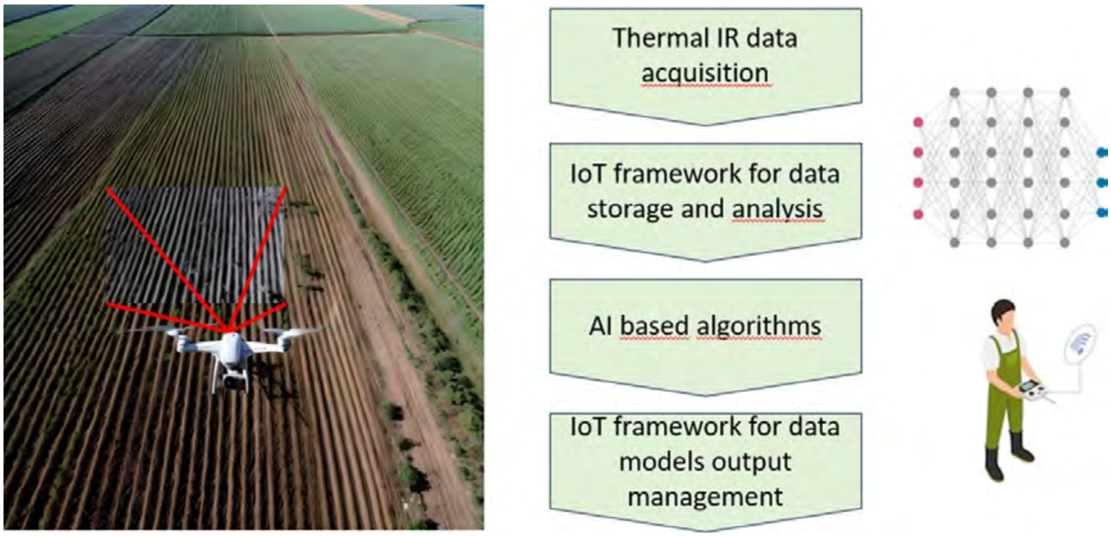

Figure 5. A possible technological hub integration for agriculture management. This framework encompasses the integration of IR imaging, eventually mounted on UAV, with AI and IoT algorithms.

Thermal IR imaging has been demonstrated to be a powerful method for identifying diseases in plants because it can record temperature differences linked to pathogen infections. Research has emphasized the capacity of thermal imaging to identify and monitor plant diseases by evaluating temperature fluctuations caused by stress imposed by pathogens such as pathogenic bacteria, fungus, nematodes, and viruses [70, 71]. Moreover, thermal imaging has shown potential in identifying the ripeness and quality of fruits and vegetables in agriculture and the food business [72]. Particularly, thermal IR imaging has been employed to discern various phases of fruit ripeness, particularly in unblemished tomato fruits [73], but also to identify excellence of fruits, as well as identifying injuries in fruits and vegetables [74].

Advances in science and technology to meet challenges

Concerning a spread and proper application of this technology in agriculture, it is worth to highlight that some limitations should be addressed and overcome. For instance, the accuracy of thermal imagery can be affected by environmental factors such as weather conditions. To meet this challenge, it is essential to allow the camera to acclimatize to local weather conditions, and to protect it with a casing in order to reduce air temperature effects on the sensor when mounted on UAV [75]. Moreover, algorithms that can adjust the data for weather influences should be developed. Another relevant issue is related to the data management. In fact, handling the vast amount of data generated by thermal imaging can be challenging, hence data management systems should be implemented exploiting IoT solutions. Concerning the improvements of the sensors and data analysis, it should be highlighted that a good spatial resolution should be provided by IR cameras when they are mounted on an UAV. In this perspective, more sensitive optics should be developed, and algorithms able to generate fine spatial resolution thermal images from coarse spatial resolution [76]. To this aim, also the integration of IR imaging with other techniques could help to overcome this limitation. In fact, combining thermal imaging data with geographic information system (GIS) can help in mapping and monitoring the spatial variability of crop fields, aiding in more precise agricultural planning and management [77]. Moreover, the employment of AI algorithms could aid in enhancing the quality of thermal images, by filtering noise and improving the clarity, which could lead to more accurate analysis [78]. AI could also help automate the data analysis process, saving time and reducing the workload on farmers. Moreover, AI models able to forecast crop yields or identify potential pest infestations before they might produce significant problems could be developed. AI can help in the implementation of PA, where farmers can make data-driven decisions to manage their crops more efficiently, and it can facilitate remote monitoring of crop fields, allowing farmers to detect issues without having to physically inspect the fields, thus saving time and resources. In addition, AI systems can provide real-time alerts for potential issues detected through thermal imagery, helping farmers take timely actions to prevent losses. A possible technological hub integration is proposed in figure 5.

Concluding remarks

IR thermal imaging has the capability to delineate subtle variations in temperature, providing several advantages in agriculture. The most relevant applications of such a technology are related to detect plant stresses even before physical symptoms manifest, evaluating the condition of the soil, to manage the irrigation and to detect bruises, thereby heralding an era of preventative and proactive agriculture management. Leveraging advancements in sensor technology, coupled with the integration of AI, can potentially morph the current challenges of the employment of thermal IR imaging in agriculture into catalysts for further innovation, paving the way for intelligent agricultural solutions characterized by automation, predictive analytics, and real-time monitoring.

4. *In-situ* fluorescence responses for agriculture

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Status

Chlorophyll fluorescence is a phenomenon based on the ability of chlorophyll molecules in the plants and algae to release a part of absorbed energy in form of light emission at specific wavelength. This release of absorbed energy is in direct competition with heat dissipation and with the photosynthesis process. Fluorescence measurements can be classified as passive (*e.g.* natural sunlight) or active excitation methods. Both passive [79] and active [80, 81] chlorophyll fluorescence measurement methods have been investigated using unmanned aerial, ground and manual systems [82]. By analysing the fluorescence emission light, the physiological status, stress level and environmental interactions of plants can be retrieved at different scales [83].

At the leaf level, chlorophyll fluorescence measurements allow the analysis of the plant photosystem II efficiency (*i.e.* conversion of absorbed light energy into chemical energy). Key parameters can then be extracted, among them, the effective quantum of the photosynthesis process [83]. Furthermore, these measurements have informed on the ability of plants to manage the absorption of light under various stresses, either biotic or abiotic [84].

At the plant scale, the global health of the whole plant has been estimated through the stress-induced changes in fluorescence patterns [85]. In addition, the photosynthetic capacity and efficiency have been studied at different phenological stages. Moreover, depending on the environmental conditions, the fluorescence response can provide information on the adaptation of plants to their surroundings [86].

At the canopy level, chlorophyll fluorescence has been used to probe the photosynthetic activity (PSA) over a large area and to reveal changes in ecosystem dynamics (*e.g.* responses to climate change and shifts in plant communities) [79]. Also, it allowed to map stress patterns for assessment of regional environmental conditions as well as potential agricultural or ecological challenges (figure 6).

Plants organs contains not only chlorophyll molecules, but also several other pigments (*e.g.* carotenoid, anthocyanin, and flavonoid). They play a role in metabolic processes such as flowering, light harvesting and photo-protection. These other pigments can also provide information about daily and weekly regulation processes but with a lower quantum capacity than chlorophyll molecules. Thus, the chlorophyll fluorescence signal must be strongly reduced to detect the pigments' emission. For this, field and indoor systems have been developed, enabling the detection of chlorophyll-fluorescence-compensated signals. The physiological interpretation of fluorescence signals from pigments other than chlorophyll has been useful to determine some stresses which do not impact the PSA [87].

Current and future challenges

Plant physiology studies are generally conducted in controlled environments such as greenhouses and growth chambers [82, 88], to constrain most of experimental conditions. By conducting these studies outdoors using agro-equipment and automated platform [82, 89], it would be possible to investigate the influence of the natural environment on the complex response of genetics features to real agricultural management practices [90].

In the field and indoor, active chlorophyll fluorescence can be measured at the leaf scale using a leaf clip. At the plant and canopy scales, a phenotyping cabinet or a robot-mounted sensor can also be used. However, the duration of a full protocol of chlorophyll fluorescence active measurement is currently too long for high throughput plant phenotyping. To cope with this limit, the instruments thus require low photon noise and, when performed outdoor, low wind to avoid any leaf motions [89]. Greater integration of fluorescence measurement systems on field robots would increase the measurement throughput over agriculture experimental or production fields.

In addition, the influence of the leaf angle on the chlorophyll fluorescence signal is currently not fully considered. A fluorescence measurement combined with a geometric distribution of the canopy would enable the determination of the spatial distribution of PSA over the canopy [91].

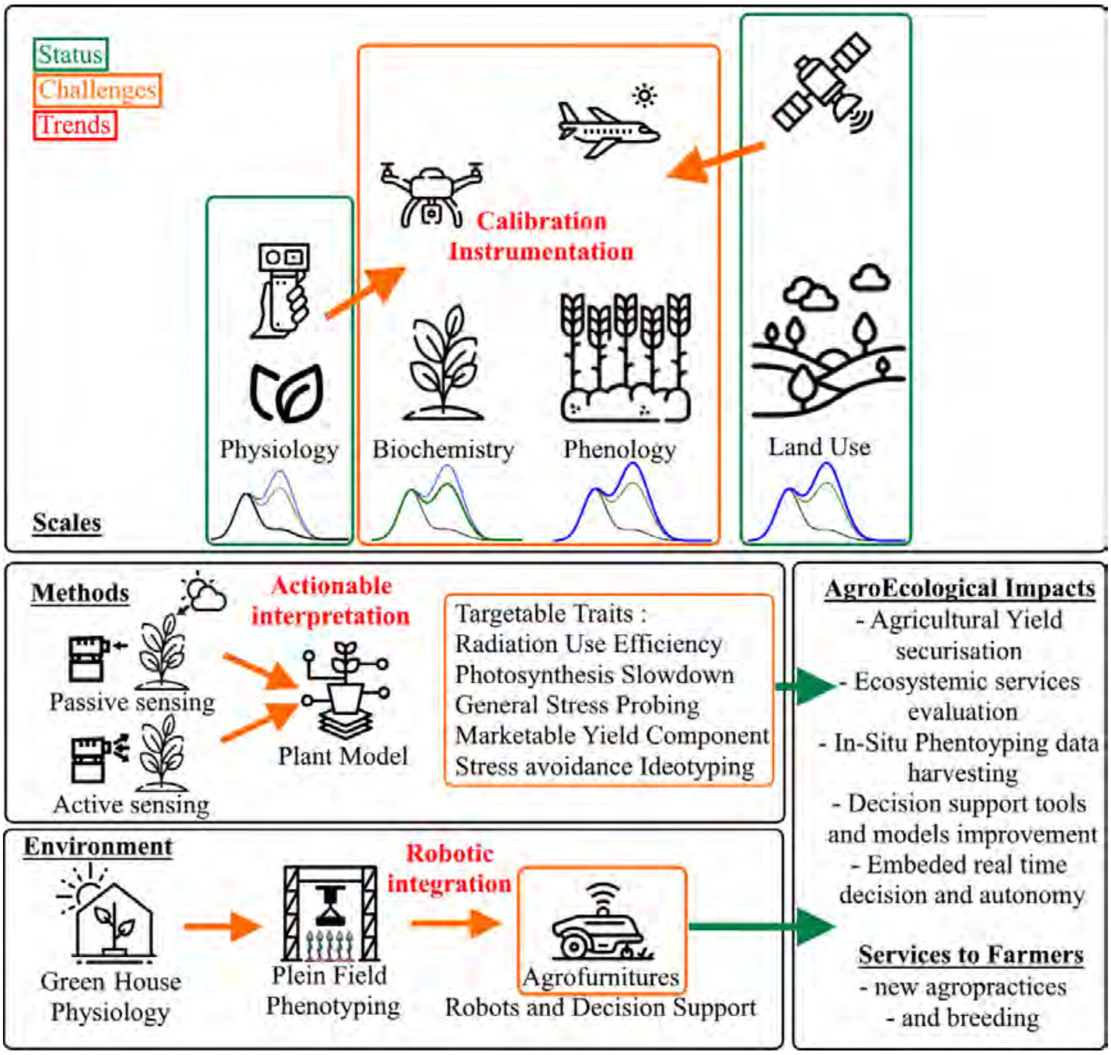

Figure 6. Representation of scales(top), method (middle) and environmental (bottom) established status (in green), current challenges (in orange) and trends of progress (in red) among the community for a broader use of plant fluorescence. This figure has partly been designed using images from Freepik.com.

Active and passive measurements of the chlorophyll fluorescence provide complementary physiological information. Until now, the different measurement protocols, instruments and correlation of their signals are not yet compatible. Thus, instrument calibration and data fusion from different measuring methods stay a major challenge [92].

Chlorophyll fluorescence signals need to be accurately interpreted to obtain a quantitative estimate of the plant phenotyping traits, as well as for their physiological significance. For example, physiological imaging performed outdoor could significantly contribute to a better understanding of the spatial distribution within the canopy of the radiation use efficiency (RUE) [93]. RUE is an indicator that quantifies the ability of plants to convert solar radiation into biomass. Fluorescence-based physiological imaging could reveal the spatial distribution of PSA over the canopy, the impact of stress conditions and environmental interactions on the RUE, the influence of the canopy structure on the light penetration and the light-to-biomass conversion. Moreover, long-term outdoor studies of RUE could be conducted, leading to records of temporal dynamics of light with seasonal variations [94]. These experimental measurements could then improve RUE-assisted models for simulating plant growth and crop productivity.

At the cellular scale, biochemical, anatomical and ontogenetic properties of leaves could be investigated [95]. Interpretation of these results would allow to better understand the microscopic origins of the *in-situ* macroscopic behaviors of leaves parameterized by environmental interactions and photosynthetic properties. For this, handheld fluorescence microscopes should be developed for field use.

Pigments other than chlorophyll are easily detected and analyzed using leaf clips. However, outdoor acquisition of fluorescence signals of these pigments using contactless tools seems difficult due to their low emission intensity and overlapping emission spectra [87].

Advances in science and technology to meet challenges

Recent advances on phenotyping platforms have allowed to quickly and automatically collect morphological and physiological traits of plants in the field [82]. Further increasing the acquisition rate of chlorophyll fluorescence signals would be beneficial for breeding (i.e. selecting cultivars for their tolerance to different stresses [96]). Nowadays, a multitude of instruments are embedded on these robotic platforms, such as RGB and hyperspectral cameras, or even lidar sensors. Eventually, they will be used to retrieve the orientation and height of the leaves and data from optical sensors will be combined, reinforcing the concept of multi-sensor data fusion [97].

Recent technological advances in illumination (*e.g.* laser diode) and collection (*e.g.* fast avalanche photodiodes and cameras) components appear promising for chlorophyll fluorescence measurements. Indeed, they will not only make it possible to increase the acquisition rate, but also to improve the signal-to-noise ratio of measurements in the field. These advances will minimize the influence of sunlight that occurs at the leaf, plant and canopy levels. Furthermore, in some applications, high optical power sources will allow to saturate the photosynthesis process activated by the absorbed light energy. The working distance (currently around 70 cm) and the measurement area (currently around 1 m^2) [89] will thus both be increased.

Harmonic analysis of chlorophyll fluorescence in plants is a novel method based on the decomposition of the fluorescence signal into its harmonic components, providing a more detailed and nuanced assessment of the various physiological and photochemical processes occurring within photosynthetic organisms [98]. The advantage of harmonic analysis lies in its ability to disentangle different physiological processes that contribute to the overall chlorophyll fluorescence signal. By analysing the amplitude and phase relationships of these harmonics, one can better understand the dynamic responses of photosynthetic systems to changing environmental conditions, stressors, and various regulatory mechanisms.

Recently, the use of sensor-plants has been investigated on detached leaf in controlled-environment laboratories [99]. These genetically modified plants produce specific fluorophores when they are exposed to specific stresses. At given phase and amplitude interrogations, these fluorophores generate specific fluorescence signals, improving the early detection of stresses.

Concluding remarks

Chlorophyll fluorescence is a promising optical technology, enabling to retrieve crucial *in-situ* information in agriculture, such as the health, physiological status and environmental interactions of crop plants. Optical and robotic advances do not yet permit high-throughput phenotyping fluorescence measurements in both passive and active excitation modes. Integrated in numerical models, they enable improvement in crop productivity and they strengthen the capacity to adapt to climate change. In addition, studying the *in-situ* behavior of leaves at the microscopic scale is needed to understand environmental interactions and photosynthetic properties.

Acknowledgments

This work was partly funded by a National Association for Research in Technology (ANRT, France) Grant [No 2022/1856] and a FEDER (Fonds Européens de Développement Regional) [No EU001292] Grants. The authors thank both the Biophotonics Team of Photonics Bretagne and Department of Crop Phenotyping of Arvalis which contributed to the work described in the section, as well as Dr Gwenaëlle Lefeuvre for their constructive contribution to the drafting of the manuscript.

5. Hyperspectral imaging applications in the agri-food sector

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Status

HSI is an advanced detection technique allowing to acquire the spectral reflectance associated to each pixel of the image [100]. HSI dates to the late 1970s when it was developed by NASA's Jet Propulsion Laboratory. Originally utilized in several remote sensing applications, in the last year's it has been made available for laboratory, industrial and 'ground-based' applications. Hyperspectral devices acquire hundreds, or even thousands of spectral bands, at very narrow intervals across the electromagnetic spectrum. In agri-food sector the spectra range usually spans between the ultraviolet (UV) (100–400 nm) and the SWIR regions (1000 and 3000 nm), passing through the VIS–NIR (400–1000 nm), representing these intervals the right balance between meaningfulness of the acquired data and device costs [101]. Following this approach, and starting from the collected spectral signatures, several actions can be performed, they are synthetically reported in the following:

- *crop health monitoring*, for disease early detection (i.e. fungal infections), or nutrient deficiencies, as well as water stress and pest infestations, thus allowing to adopt timely and correct pest control, irrigation, and fertilization strategies, thus minimizing the environmental impact [102, 103];
- *weed detection*, through the distinction of crop plants and weeds according to their spectral signatures [104];
- *soil analysis*, allowing to define maps embedding information on soil composition, moisture content, and nutrient levels across a specific area, to be used in precision farming for a rational and sustainable use of fertilizers and conditioners, reducing waste and improving soil health [105, 106];
- *fruit and vegetables harvesting quality*, detecting and quantitatively assess bruising, ripeness and defects (figure 7) [107–109];
- *food quality assessment,* real-time detection and identification of contaminants, foreign objects, or spoiled items inside the food manipulation chain for safety and process control [110].

All the previous mentioned actions will be object of further development not only through the *improvement of sensing devices*, and *strengthening detection architectures*, but also *implementing AI based logics*, instead of the chemometric approaches [111], currently adopted for data handling, analysis and consequent recognition/classification algorithms set up. Chemometrics, in fact, even until today remains a powerful analytical tool, presents some potential 'practical/operative' disadvantages mainly linked to the required sophisticated algorithms and computational power, the existing intrinsic lack of HSI knowledge and integration inside the existing agri-food systems and practices, the access to HSI technology especially in developing countries, the need to adopt standardized protocols, to collect, analyze and interpret data and, finally, the need of an extensive education and training.

Current and future challenges

It is well known as HSI is powerful tool to acquire detailed information about crops status, soil composition, and quality of agricultural products (figure 8) [112]. The potentialities of HSI as a link in the different agri-food sector production/control stages, even if correctly addressed, have not been yet fully explored and implemented, especially with reference to the field. Current and future challenges are related to the development of further analytical and technological approaches and the resulting implementations.

- Analytical and technological developments will be mainly addressed to:
  - *Acquisition architectures* (i.e. satellites, drones, handheld, or fixed units) [113] are expensive to acquire and maintain and can represent a barrier for smaller farms, thus they cost decrease represents one of the main future challenges.
  - *Miniaturization*, allowing an easier integration inside already existing operative units and platforms. The fulfillment of this goal will enable a larger utilization of HSI detection and analytical approaches [114, 115].
  - *Development of hyperspectral sensors characterized by higher spatial and spectral resolution* will allow to acquire more detailed and accurate information about crops, soil, and other agricultural elements [116].

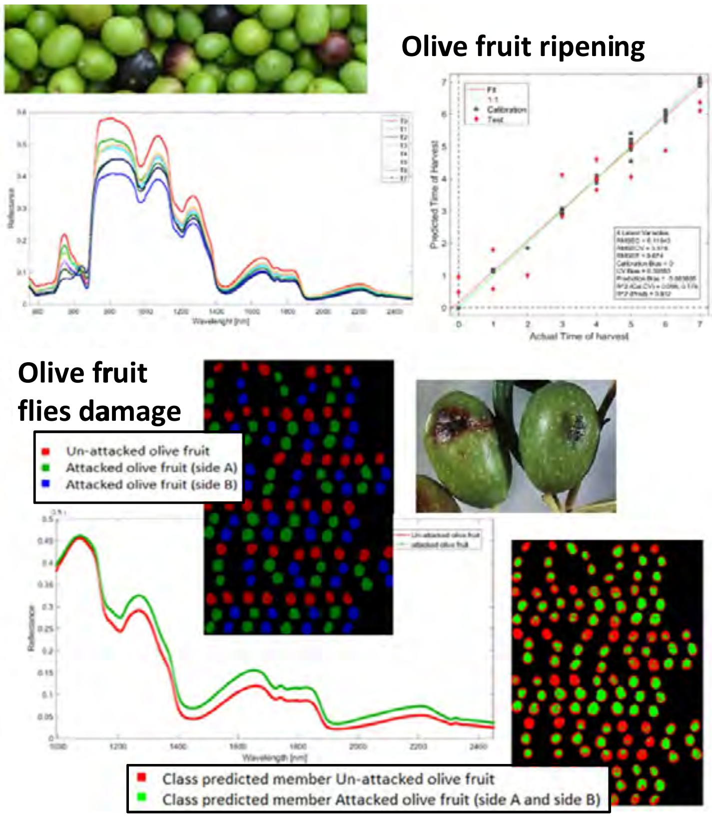

Figure 7. Examples HSI based analytical strategies applied to olive fruit ripening and olive fruit flies (*Bactrocera oleae*) damage. Average reflectance spectra of olive fruit characterized by different degree of ripening (a) and attacked and un-attacked by mosquito fruit flies (b). Olive ripening prediction following a partial least squares (PLS) regression (c) and results of partial least squares discriminant analysis (PLS-DA) classification for damaged an undamaged (d) olive fruit. Reproduced from [107].

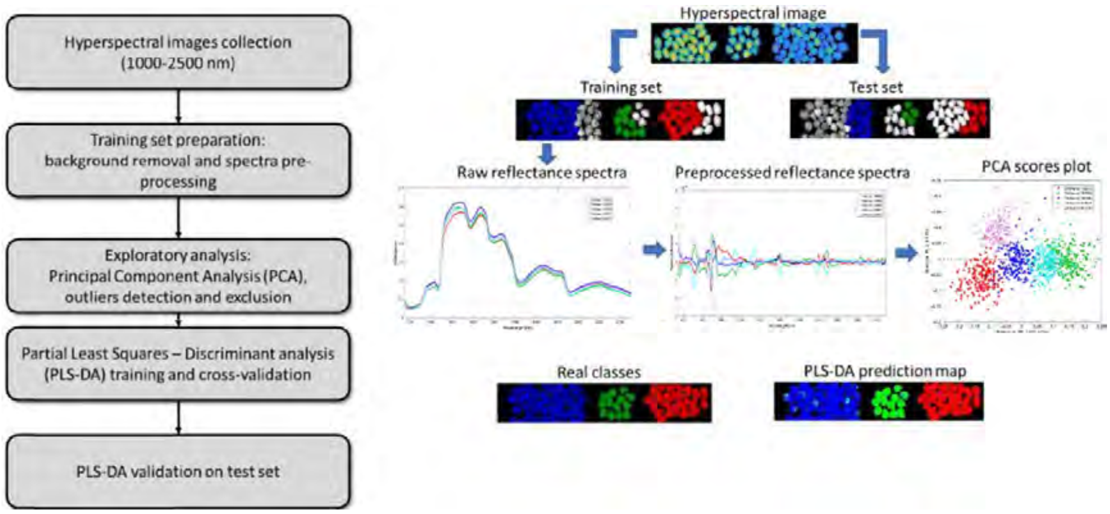

Figure 8. Examples of strategies, procedures, and results to perform agricultural products quality assessment following an HSI based approach [112]. Preliminary to classification set-up, hyperspectral images are pre-processed performing a background removal. A combination of pre-processing algorithms is chosen to attenuate un-wanted occurring sources of noise, enhancing spectral differences among samples. Principal component analysis (PCA) is used as an exploratory analysis tool. Occurring outlier are successfully identified and removed from training sets used to calibrate classification models. A classification model is then applied. One of the most utilized is the partial least squares-discriminant analysis (PLS-DA). PLS-DA is a supervised pattern recognition technique. PLS-DA model is calibrated with pre-processed spectra extracted from region of interests (ROIs) depicting known samples, cross- validated and validated on a test set.

- *Data handling and analysis.* The fulfillment of the previous goals will produce as a result extensive data sets and specialized databases (i.e. hyperspectral libraries for different crops, diseases, soil conditions and, agricultural regions) requiring more sophisticated algorithms, and ML techniques (i.e. deep neural network,

DNN) to process and analyze, both in terms of quantity and quality, this huge amount of information [117, 118].
    - *Customized hyperspectral solutions*, tailored to specific agri-food applications, (i.e. pest detection, nutrient assessment, presence of bruise and/or molds, etc).
- Applications could be strengthened in many fields as:
    - *PA*, performing a stronger integration with GPS and drones to optimize resource use, reduce environmental impact, and enhance the overall crops efficiency.
    - *Sensor based irrigation systems*, allowing automated watering and oil moisture monitoring.
    - *Vertical farming*, adopting sensing architecture, and related HSI based control logics, in hydroponics, aeroponics, indoor lighting control, allowing year-round production, reduced soils consumption and productions waste minimization.
    - *Automation*, HSI driven robots for planting, harvesting and weeding actions.
    - *Waste identification and classification*, allowing finalized agricultural by-products reuse in a circular economy perspective.

Finally, farmers and agricultural professionals' acceptance and education on the applications and interpretation of hyperspectral data, together with the introduction of new legislative rules and protocols, considering HSI base strategies, are fundamental for future successful and sustainable HIS based applications.

Advances in science and technology to meet challenges

The advances in science and technology, influencing the agri-food sector, will necessarily have to consider climate changes which will increasingly affect the methods of cultivation and handling of products. The development of technologies capable of supporting the control and evaluation of the state of crops in controlled environments (i.e. greenhouses) will certainly become increasingly important, also thanks to the fact of being able to operate in environments where the variability of abiotic factors is minimized. HSI, in such environments, will be able to strongly contribute to the overall optimization of cultivation processes. In this perspective some factors assume preeminent importance, that is:

- *Devices miniaturization*. Compaction of the optics (i.e. mirrors, lens, and filters), components integration (i.e. energizing source, detectors, and spectrometers) and microscale sensors development are three aspects of paramount importance to reduce not only dimensions but also weight, energy consumption, costs and, at the same time, increasing the possibility of HSI device integration in already existing analytical architectures, and/or customization for specific new applications. The fulfillment of this goal will allow a larger utilization of this technology.
- *Data processing improvement,* that is the possibility to implement 'on-board' advanced algorithms and signal processing to handle and analyze data or performing 'real-time' remote analysis, transmitting the acquired data, and receiving the result through wireless connectivity. Following this approach, the 'remote integration' with other devices can also be realized.

Both the two factors will contribute to facilitate collaboration, and the advanced scientific understanding, thanks to the possibility to share data at local scale on crop health, nutrient levels, and water requirements or, at larger scale, on diseases and pest monitoring, thus allowing to define and set up shared intervention strategies among the different subjects involved (i.e. farms, cooperative, agri-food industries, food distributors, local, regional or national authorities), optimizing efforts and resources. Data sharing, if from a scientific and a technical point of view presents great advantages, generates, on the other hand, the need to define clear rules on data ownership and a their correct and ethical 'shared' utilization.

Concluding remarks

The use of HSI in the agri-food sector will play more and more an important role also in an Industry 4.0 perspective. Specific database can be generated and utilized embedding information to utilize to develop comparative evaluation logics (i.e. big data handling/analysis) for a better and faster understanding of new occurring phenomena and/or new process results. Furthermore, it will be necessary to define a sensory-based IOT information architecture where the HSI based information represents the core to define other possible investigation tools, both hardware and software providing information that can be aggregated, stored, and analyzed for more elaborate and holistic reasoning and inference. Finally, the data collected to produce elemental mapping related to crop and products evolutionary status could be also profitably handled using ML algorithms (i.e. DNN) finalized to perform their classification generating knowledge specific on crops growing and cultivation characteristics in a certain area, in respect of different environmental conditions and variables. Finally, device miniaturization and players awareness will be the other two important aspects that in the next years will strongly influence the application of HSI in the agri-food sector.

Acknowledgments

This study was carried out within the Agritech National Research Center and received funding from the European Union Next-GenerationEU (PNRR—MISSION 4 COMPONENT 2, INVESTMENT 1.4—D.D. 1032 17/06/2022, CN00000022—CUP: B83C22002920007). This manuscript reflects only the authors' views and opinions; neither the European Union nor the European Commission can be considered responsible for them.

6. Digital twin for smart multispectral camera design

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Status

Spectral imaging allows seeing subtle optical signatures or light wavelengths invisible for human vision. This has potential for numerous industrial applications and a large economic impact by improving quality inspection, increasing automation and the development of innovative applications. Consequently, spectral imaging has become an active field of research in the world, illustrated by the many companies (e.g. Specim, Headwall, etc) and research institutes (IMEC, Flanders Make, etc) involved in this topic via basis research or hardware design and exploitation. Industrial applications can already be found in food sorting, recycling, medical and remote sensing [119]. On the other hands, recent advances in ML algorithms boost the target detection (identify specific objects in your product in real-time), quantification (measure the composition percentage of a component in your product) [120]. DTs are helping the manufacturing industry work smarter and more efficient [121]. By combining the spectral camera and ML methods, one can exploit DTs to optimize the configurations of camera design, decrease downtime and the cost, then perform continuous and automatic quality inspection on your food production line based on chemical analysis (by using the designed camera). This provides a non-destructive solution for chemical analysis and can be integrated with other modules (e.g. machine control and sorting systems), greatly reducing manpower in the production line, as well as increasing the efficiency.

Current and future challenges

Popular commercially available hyperspectral solutions employ a push-broom approach combined with a grating and a silicon or InGaAs sensor to record the spatial-spectral signal, as shown in figure 9. Solutions that combine multiple sensors can cover wide wavelength ranges. State of the art examples are the Headwall photonics Co-Aligned VNIR-SWIR imager, with a spectral range in the VNIR + SWIR (400–2500 nm), obtained by splitting a single line into two spatial-spectral signals on a silicon CMOS and a mercury cadmium telluride sensor, or the popular Specim FX17 SWIR linescan sensor based on a InGaAS sensor, sensitive in the 900–1700 nm range [115]. When area images are desired, the state-of-the-art solutions employ selective illumination, filtering, or spatial-spectral patterns. An example of the solution (spatial-spectral patterns) is the IMEC sensors, a pixel array based on Si or InGaAs technology is overlayed with a band-pass filter pattern. Interpolation of each band to the full resolution is required and can introduce artifacts.

An alternative is to employ multiple camera systems, each with its own filter. This often results in relatively low-cost solutions for multispectral imaging systems, and is a popular solution for e.g. drone applications and index-based approaches. Alignment of the different images can then become an issue. This issue can be avoided by using a single camera with a rotating filter wheel, but this defers the alignment issue to the temporal instead of the spatial domain. A common challenge in the development and deployment of such industrial spectral imaging systems is the multitude of design decisions that have to be resolved, and the prior unknown performance of the resulting device for a given industrial processing task. A concrete example is the choice of spectral bands that will be integrated in the device. Depending on the technology, a number of bands can be used, e.g. by choosing the filters in a filter wheel or on a number of parallel cameras. The resulting spectral image can then be used for further processing, but obviously the design choices and algorithm details influence the performance of the desired task.

Advances in science and technology to meet challenges

The design of smart spectral cameras that are optimized for solving certain tasks (e.g. target detection, classification, quantification) is in high demand in industry. As optimization exclusively with respect to task performance would often lead to infeasible or very expensive designs, a trade-off must be included that takes design complexity and price into account. Many technological approaches (as shown in figure 9) can be followed to obtain spectral signals or images, each with its own advantages, drawbacks, constraints and price point. To build a design space for spectral cameras, several topics must be addressed:

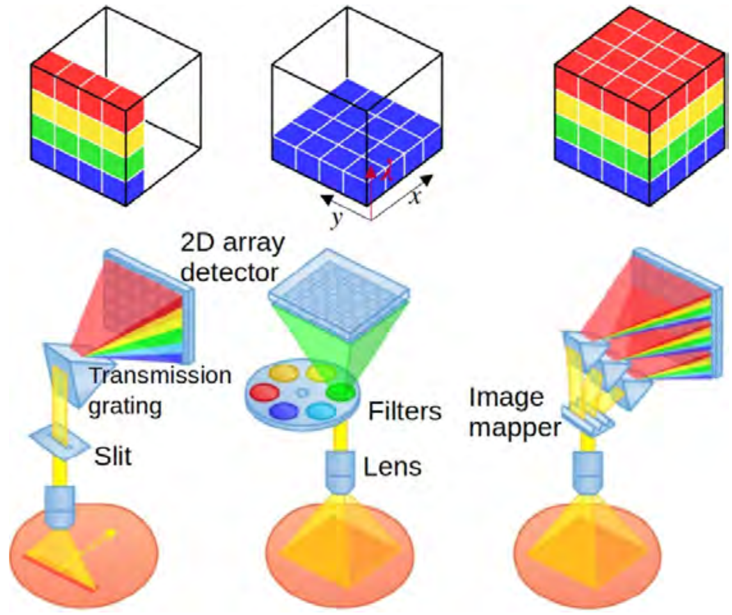

Figure 9. Left: push-broom system with spatial-spectral decomposition via grating [122]; middle: spectral imaging via variable LED illumination and/or tunable optical filter elements [123]; right: hyperspectral sensors from imec [124], with color-coded filter patterns sensitive in the VIS–NIR range.

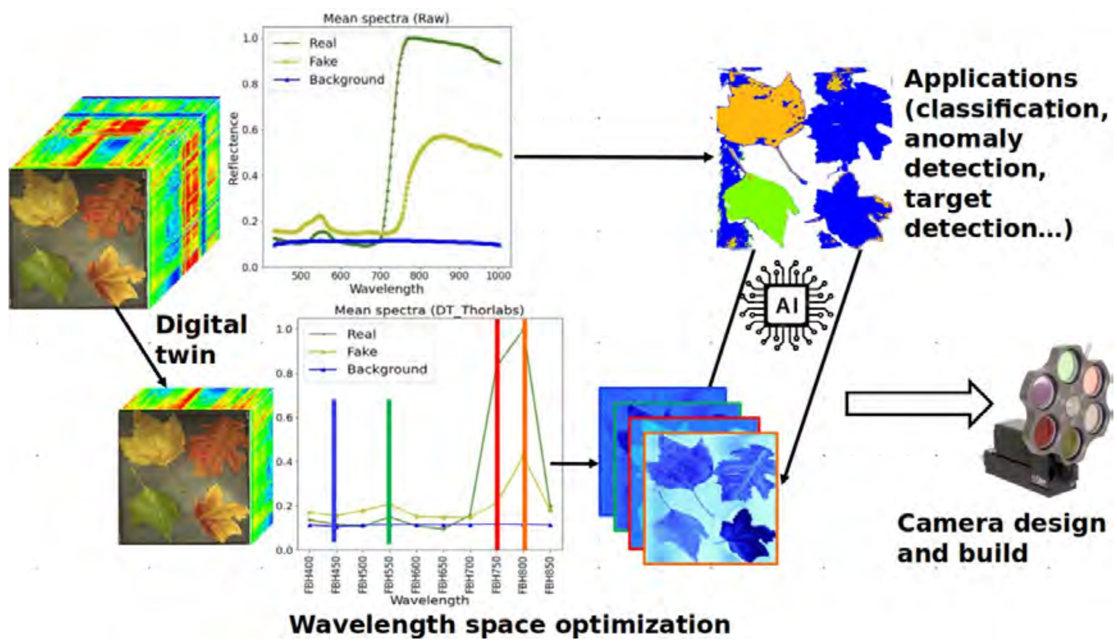

Figure 10. Task-driven smart industrial spectral camera design via digital twin and artificial intelligence (VLAIO SISCAI project) [128].

- What are the possible inputs of the space, and in which range are they allowed to vary?
- What are the constraints on the inputs? Certain combinations are not feasible.
- What are the desired outputs of the design, e.g. optical performance, price estimate, design complexity, …?
- How to model these outputs given a design space input and an 'idealized' known input?

With DT, we can build a multispectral camera in a digital way (before manufacturing a real physical camera), where a number of design choices (size, weight, power usage, processing capacity, framerate, etc.) and high-quality spectral inputs are given, a sensor or camera output signal can be simulated, as indicated in figure 10. This will allow us to find the optimal trade-off between system performance and cost. Recent AI methods will be exploited to solve this type of optimization problems [125, 126]. While many forms exist, genetic algorithms or particle swarm optimization methods have been successfully used for design space optimization [127]. These algorithms are based on swarm intelligence, and iteratively try to improve a candidate solution with regard to the objective function by having a population of candidate solutions and moving this population around in the search-space according to simple rules (e.g. random searches or mutations, attraction to the best solution, local random search around good candidate solutions, recombining two good input sets into new input sets, …).

Concluding remarks

Fast design of a multispectral camera in a smart way (where performances and prices are well balanced) that can carry out real-time target detection, quantification, etc, is in high demand in industry. Especially for earlier disease detection of plants and real-time food defect detection, where very high spatial and temporal resolution spectral cameras are required to better characterize the tiny disease symptoms (or defects) under very complex environmental conditions. DT can facilitate the design of multispectral cameras, where all the functions/devices (light sources, lens, filters, etc.) required by the customers can be simulated before manufacturing a real physical camera. AI can find the best combination of different devices in a faster and smarter way. This way we can find the trade-off between system performance and cost. Future work will consider environmental factors (illuminations, humidity, temperature, etc) in DT, to reduce the spectral variations.

Acknowledgment

This work is financially supported by the VLAIO ICON Project (SISCAI-2021-0599): 'Smart industrial spectral cameras via artificial intelligence'.

7. TeraHertz spectroscopy application in agriculture and food technology

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Status

The TeraHertz spectral range (100 GHz–10 THz) lies at the intersection of electronics and photonics, with 1 THz corresponding to a timescale of 1 ps, an energy of 4 meV, and a wavelength of approximately 300 μm (figure 11). THz spectroscopy is a non-destructive and non-invasive technique, well-suited for potential food processing and inspection applications due to the following properties. THz waves are non-ionizing and penetrate many common packaging materials, such as paper, cardboard, and plastic. These advantages have motivated numerous research studies in food science and agriculture involving THz spectroscopy. However, it is still a relatively recent technology and is in its early stages of development.

Historically, the so-called THz gap posed a challenge due to the high cost and limited efficiency of available emitters and detectors. However, advances in the 1990s greatly improved the feasibility of THz applications. Electronic sources, like multiplication chains and vector network analyzers (VNAs), now operate beyond 1 THz, offering extremely high signal-to-noise ratios and frequency resolution. However, these systems are expensive, with costs often approaching €1 million. Such precision makes them ideal for standardization. Meanwhile, advances in photonic sources, including time-domain spectroscopy (TDS) and continuous-wave frequency-domain generation, have enhanced accessibility. These methods rely on laser-based optoelectronic conversion and have progressively improved in performance, compactness, and affordability, with system costs now often below €100 000. This cost reduction and technological refinement have made THz spectroscopy increasingly viable for real-world applications and further integration into commercial instruments.

While THz spectroscopy's capabilities for non-invasive, remote sensing applications in food science and agriculture are promising, it remains in the academic phase of development. Current studies employ THz spectroscopy to investigate the picosecond-scale dynamics in solid, liquid, and gaseous states [129]. For instance, THz methods have been explored to monitor molecular crystal crystallization during sugar processing, detect adulteration in liquids, and identify volatile compounds in gases. However, to date, none of these applications have reached the industrial implementation stage, underscoring that THz technology's readiness for practical use in agronomy and food technology is still nascent.

Current and future challenges

THz spectroscopy approaches in agrifood have been developed for applications across the three phases of matter: liquids, solids, and gases.

For liquids, THz spectroscopy leverages the strong broadband absorption of polar solvents like water, which has a significant absorbance in the THz range (e.g. $\sim$200 cm^{-1} at 1 THz). This absorption is highly sensitive to changes in physical or chemical parameters, such as temperature or composition such as the temperature or the composition, making THz spectroscopy a powerful tool for detecting compositional variations in liquids, such as measuring carbohydrate concentration [130] and detecting adulteration in products like acacia honey [131].

In solids, two main THz approaches are utilized. The first approach uses water's high absorption to monitor moisture levels in samples. In this application, samples absorb more THz radiation as their water content increases, enabling effective monitoring of food and agricultural products for evaluating drought stress in plants [132] or general moisture content. The second approach targets molecular crystals, such as carbohydrates, which exhibit specific THz signatures influenced by both molecular conformation and crystal structure [133]. Applications have included studies about detecting melamine in milk powder [134] motivated by the poison milk powder scandal, measuring flavonoids in waste orange peels [135], and assessing protein content in soybean powder [136].

For gases, THz spectroscopy is highly selective for volatile organic compounds (VOCs) [137]and is particularly suited for analyzing complex VOC mixtures in food and beverages, with potential applications in quality control for aroma profiling and safety monitoring. Advances in THz technology have improved sensitivity, allowing for detection of gas-phase contaminants at the ppm level [138]. Applications include ammonia detection in storage and transport settings (as reviewed in [139]), as well as microbial monitoring through gas by-product analysis. Recent THz spectroscopy advancements have achieved sensitivity levels

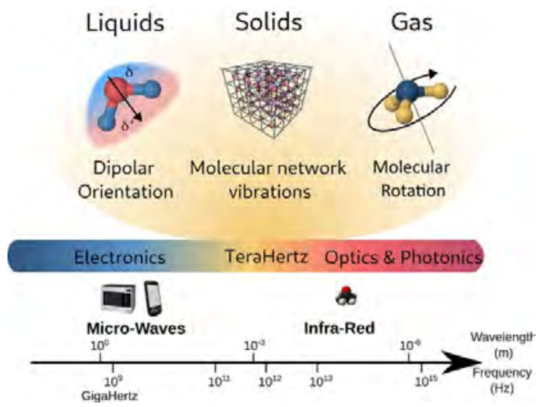

Figure 11. TeraHertz spectroscopy probes material in the liquid solid and gaseous phase. Maturity of the approaches differ with the phase but each of them can be used for agriculture and food technology depending on the application.

comparable to SIFT-MS for detecting H_2S contamination in packaged Atlantic salmon (Salmo salar) [140], using cost-effective ultra-high-frequency electronics.

Advances in science and technology to meet challenges

The cost and performance of THz systems are crucial factors for their adoption in the agrifood industry. Since THz components and systems are still emerging, performance is steadily improving, and costs are expected to decrease with broader adoption, although certain applications remain beyond immediate reach. A major research focus is on achieving sub-ppm sensitivity without compromising compactness. One promising approach is extending the optical path within gas cells, either through multipass configurations or resonant techniques. A circular gas cell, for instance, can enhance the optical path length by 20 times [141], while ultra-high-finesse Fabry-Pérot cavities, relying on specialized quasi-optic methods such as low-loss corrugated waveguides with highly reflective photonic mirrors, now reach finesses above 3000. This enables effective path lengths of up to 1 km within a 48 cm cell, allowing detection of polar molecules with line strengths as low as 10^{-27} cm^{-1}/(molecule cm^{-2}) [142].

In terms of practical applications, no current methods assess the freshness of packaged food without opening the package—a significant gap THz spectroscopy has the potential to address. Current THz spectroscopic systems are too expensive and bulky to fulfill the needs of this application. One solution is integrating THz systems with micro/nano technologies. Micromechanical systems (MEMS) are a mature technology that has driven innovations across fields such as photoacoustic spectroscopy. From a more general perspective, one is witnessing a trend where the leverage offered by MEMS is solving a number of key challenges in THz applications. Examples range from MEMS-based THz detectors, reconfigurable switches and filters, and tunable biosensors [143–145]. Besides mechanical microtuning of THz MEMS-metadevices, MEMS principally enhance THz devices by transducing an electromagnetic absorption into a mechanical nano/micro-motion. As such they are highly sensitive transducers, converting photoacoustic signals to electrical ones, as already proven in infrared applications [146].

THz photoacoustic gas spectroscopy is an emerging technique that has the potential to revolutionize food safety and quality control by providing a detectorless, compact, and non-intrusive way to detect trace gases in food packaging. MEMS transducers can be integrated into the packaging material and fabricated cost-effectively using CMOS foundry wafer scale techniques. Although sensitivities in current systems are limited [147], advancements in resonator-enhanced MEMS systems [148, 149] are expected to improve trace gas detection at atmospheric pressures (figure 12). Further sensitivity gains may also come from coupling the system with photonic modes in photonic crystals using advanced concepts like topological photonics or bound-in-continuum (BIC) modes.

Finally, data processing for THz spectroscopy, though still developing, has already shown potential with super-resolution techniques for TDS [150] and more rigorous fitting approaches [151, 152]. The integration of advanced data analysis, particularly ML, is anticipated to enhance sensitivity and leverage THz spectroscopy's high selectivity for complex, real-world applications.

Concluding remarks

THz spectroscopy has only recently become practical for research applications beyond its initial community, driven by advances in THz source and detector technology. These advances will continue spurred by 6G and future telecommunications needs, as well as continuous improvements in short-pulse laser sources. Several

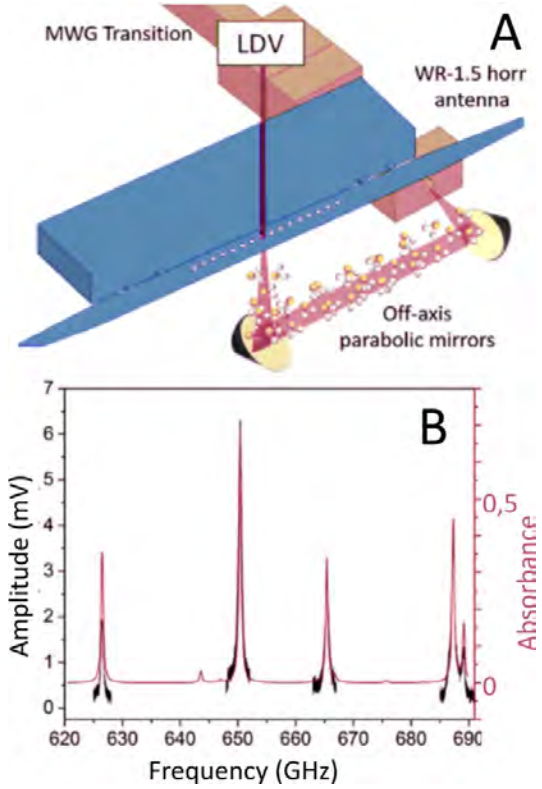

Figure 12. Example of the combination of a MEM's and THz technology proposed in the TERAFOOD project (https://terafood.iemn.fr/). An integrated THz 1D THz photonic crystal cavity combined with a MEM's sensor to probe trace gas for freshness sensing.

challenges remain before THz spectroscopy can fully meet real-world demands in the agrifood industry. Nonetheless, we are confident that current efforts to enhance the sensitivity, compactness, and integration of THz systems—along with modern advancements in signal and data processing and complementary technologies like nanophotonics and microfluidics—will pave the way for this technology's widespread adoption across the agrifood sector. From field to supermarket, THz spectroscopy holds the potential to establish new standards in food quality control, safety assessment, and process monitoring, for both gas-phase and solid-state applications.

Acknowledgments

N O and R P are grateful to the Région Hauts de France for the funding of the DEUS MAROONER project, M V thanks INTERREG France-Wallonie-Vlaanderen TERAFOOD and R P the ERC TUSCany 101089040.

8. THz sensing in agrifood: towards optimization of agricultural resources and industrial processing of food

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Status

Nestled between microwaves and infrared radiation, the terahertz (THz) range of frequencies (commonly considered as 100 GHz–10 THz) was mostly underutilized until the very end of the previous century, for both sensing and imaging purposes, due to limited availability of sources and detectors [153]. A combination of attributes including spectral specificity for a variety of molecules, high sensitivity to liquid water, non-ionizing radiation with very low energy photons, limited transparency through dry packaging materials, and greater imaging resolution than mm-waves, makes THz waves a suitable choice for several application domains, especially agrifood sensing and imaging. As illustrated in figure 13, some of these parameters are quantified for the most useful THz band between 0.1–3 THz that is easily accessible through electronic, optoelectronic, and photonic emitters/receivers [154]. At present, in the agrifood sensing domain, THz time domain imaging (THz-TDI) has been the predominant technique for proximal sensing [155], followed by tunable THz continuous wave (THz-CW) [156], low frequency THz VNA [157] and high frequency and high-power THz-quantum cascade laser (QCL)-based imaging including laser feedback interferometry (LFI) [158]. Application areas range from hydration monitoring, soil sensing, and plant pathology to food quality monitoring, adulterant detection, and others [155]. As illustrated in figure 13, THz radiation has a penetration depth of only 100–15 μms within liquid water over 0.1–3.0 THz. This shallow depth makes data acquisition, analytics and more importantly, adaptation of models challenging. While long-range applications such as THz-Lidar or radar, especially in the range beyond 1 THz is complicated due to the very high atmospheric water vapor absorption, laboratory-scale analytical applications in genomics [159], concurrent multispectral analysis at the molecular level [160] are becoming cornerstones for precision and efficiency in recent times. The agricultural sector benefits from these capabilities in optimizing crop management, soil analysis, and resource utilization, often based on the fingerprint of a biomolecule or inorganics, but also the corresponding structural and symmetry properties with advanced data analytics beyond the numerical realm and employing more ML algorithms [161]. This trend is essentially universal for probing of biomaterials in general, of which agri-food sensing and imaging is a subset. As in the THz range, experimental acquisitions from biomaterials often produce highly complex and counterintuitive results due to the compound effects of collective excitations, multiple scatterings, surface dynamics, varying hydration potential, and other effects [162].

Current and future challenges

As highlighted in figure 13, agrifood imaging was one of the first applications shown by the pioneers of modern THz technology field in 1995 [163] and within 5 years, the first commercial THz system was available [164]. By 2006, several commercial systems were offered using THz-TDS and CW techniques. However, it was only in 2011 that the first real-time in-line THz sensor for pharmaceutical applications was deployed [165] and as of 2023, there is still no commercial user platform based on THz imaging technology that could be operated in an agricultural field/facility or as an in-line quality control system in food production. Several excellent reviews [153, 166, 167] are available that discuss various aspects of THz imaging technology in general, and some of salient advantages and limitations of this technology in the specific domain of agri-food sensing and imaging are listed below:

- ✓ THz is a non-ionizing radiation and considered to be safe even over long exposure time with low to moderate intensity to human users as well as to the commodities, such as food and agricultural products.
- ✓ Limited penetration of THz through dry packaging materials, such as, paper, plastic, cloth, jute etc.
- ✓ High sensitivity of THz range to liquid water: a natural ‘chemical tag’ in agrifood domain.

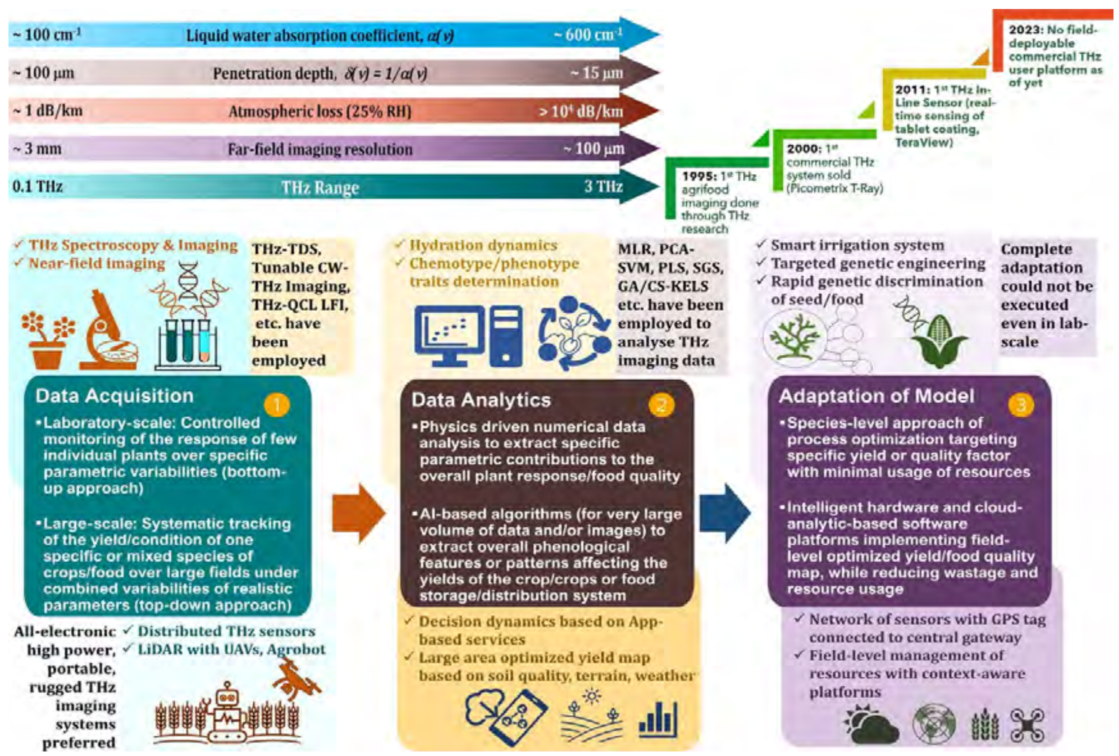

Figure 13. Important aspects of THz range sensing and imaging in agrifood sector. (Top Left) Several physical factors of THz range listed here have restricted wide applications of the same in this domain; (Down) the research landscape in agri-food domain in THz range can be divided in two specific application areas: proximal/laboratory scale and long-range/field deployable large-scale applications. In most cases, it is the former type, where both data acquisition and data analytics have matured while adaptation of the THz technology in user-end system/platform is yet to be achieved. Large-scale applications which are more suitable for industrial platform is yet to be taken up even at acquisition and analytics levels. (Top Right) The historical progression of THz field in the past 30 years has been highly asymmetric and driven by commercial interests in the domain.

✓ Better spatial resolution of THz range than mm-wave range; super-resolution imaging possible through near-field (NF) technique.

× High cost of THz imaging system relative to the value addition, in terms of specificity, sensitivity of chemical detection etc.
× Reduced limit of detection (LoD) of chemicals in THz range in the presence of liquid water.
× Slow image formation because of mostly raster scanning image acquisition techniques in vogue.
× Absence of standardized THz database of agrifood materials.

While several industry reports and reviews [168] continue to uphold very positive outlook towards the microwave and THz technology in agri-food applications, the footprint of this technology in this specific domain is still very limited compared to other traditional sensing schemes, such as, Raman, IR, HSI etc [155, 169]. While we note that AI-based analytical techniques are increasingly being employed [158, 161, 166, 169, 170] to overcome some of the challenges of the THz range mentioned above to deliver robust decision dynamics along some specific target objectives/applications, fundamental obstacles remain in this field, as discussed in the next section, which the entire THz community must address in coming years.

Advances in science and technology to meet challenges

One of the major obstacles in the path of expected and yet underachieved performance of THz technology in agri-food domain, is the absence of reliable and robust traceability of key material characterization/measurement parameters in the THz frequency range. This serious need for calibration and metrology has been mostly met in an ad hoc fashion with traditional microwave measurements reaching up to ~100 GHz, while IR techniques extending to below ~10 THz, far beyond their specified frequency range, resulting in several inaccurate, conflicting results [162]. Thus, to address this 'serious gap in information' related to metrology, other than the lingering 'THz gap in capabilities' [153] in terms of availability of basic technology enablers, the immediate critical necessity is to produce standardized databases. This work must include quantifiable THz measurements of material properties and the interactions between THz radiation and measurement systems with calibrated tools and instruments with repeatable protocols [171], especially in

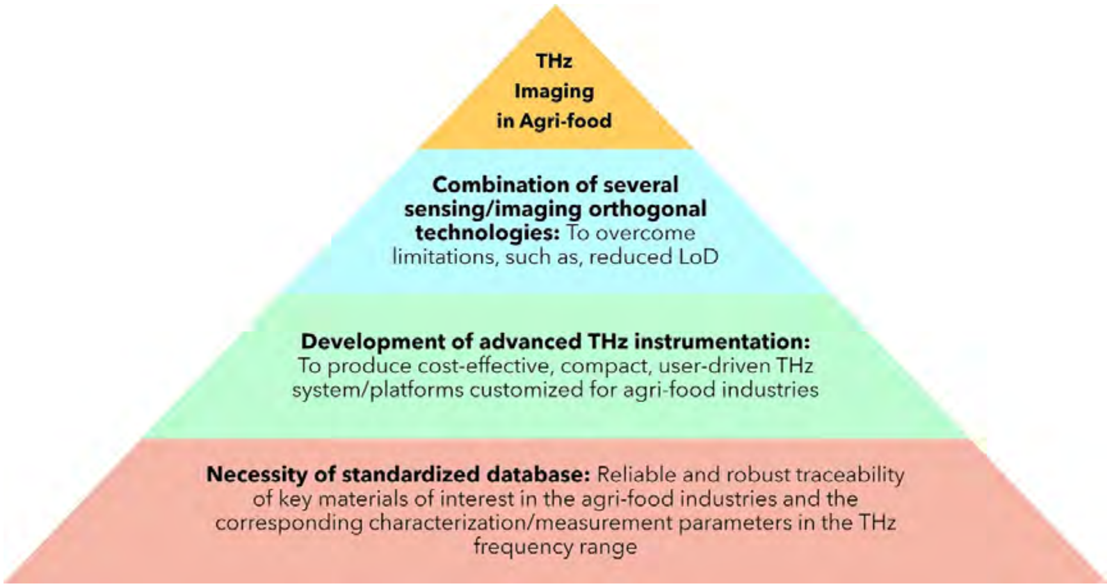

Figure 14. Key aspects of future advancements, required in the THz science and technology to serve the agri-food sector.

terms of sample preparation and handling [172]. As the entire community will have access to such a database, THz application engineers will have a greater chance of success to solve the other lingering issue: development of advanced THz instrumentation to produce cost-effective, compact, user-driven THz system/platforms customized for agri-food industries. This aspect is not only limited to the domain of agri-food but would also address the bigger cross-section of industrial applications of THz technology. In this way, one more emerging trend to solve several challenges of THz sensing, especially related to the compromised LoD of chemicals, is to develop a platform that could combine several sensing/imaging orthogonal technologies. Other than direct applicability to agri-food production and distribution, THz imaging technologies could also prove critical in shaping future schemes to reduce agri-food wastage, recycling, forming 'green' farming and food distribution practices through replacement of traditional irrigation, fertilization, and other resource-hungry practices by 'smarter' and 'more precise' assessments. It must be considered, however, that any innovative approaches of THz technologies to solve a critical problem in future is likely to be more successful when it could be implemented with the least quantum of addition and alteration to the 'traditional' structure and organization of the agricultural practices and food distribution system around the world. These key aspects of future advancements required in the THz science and technology are illustrated in figure 14 in the order of their hierarchical importance.

Concluding remarks

In recent years, application of THz sensing and imaging has experienced steep advances both in the areas of agriculture (potential to manage irrigation smartly, soil characteristics monitoring, classify seed varieties etc) and across food (potential to identify defects in production, quality control, process monitoring, testing of target pesticides/microbes/toxins in food etc) production and distribution chain [155]. And yet, this technology domain has not reached its 'promised peak' as discussed in the previous section. It is likely that with the development of diverse and novel THz-range enablers (source, detector, active and passive optics etc), techniques as well as other feeder technologies, such as, conveyor belts, robotics, UAVs etc, this technology would be able to solve several current issues: restricted LoD, slow rate of operation, higher cost of implementation, total production cost, ease of customization, data calibration and protocol standardization to establish itself as a mainstream option to enhance or complement other existing technology platforms in the domain. Moreover, a larger footprint of THz technology in future, especially in agri-food sector, is rather expected as this technology is already compatible with some of the other key emerging technologies, such as, AI, IoT, Big Data and others.

Acknowledgments

A B and A S acknowledge support from (a) Defence Research & Development Organization (DRDO) vide Grant # DFTM/03/3203/M/01/JATC, (b) Department of Atomic Energy—Board of Research in Nuclear Sciences (DAE-BRNS) vide Grant # 37(3)/14/01/2016 BRNS/37015, and (c) Department of Science and Technology—Science and Engineering Research Board (DST-SERB) vide Grant # PS-FTP/2013/78. ADR and KB acknowledge support from the Australian Research Council (DP200101948, DP21010334).

9. Lidar—remote sensing for assessments in the agro-food sector

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Status

Lasers and laser spectroscopy have developed tremendously during recent years (see, e.g. [173]). The impact in the agro-food sector has been important. Lidar constitutes one class of applicable techniques in that area. As the name implies, the most common lidar application is to transmit a short laser pulse and measure the time lapse till an echo is recorded and in that way obtain a distance measurement. Such measurements with compact sensors have recently developed tremendously for assistance in autonomous vehicle driving. Generally speaking, a lidar sensor can be mounted as a fixed installation, or it can be made mobile with a vehicle, or airborne for convenient coverage of large areas. Recent developments include wide-spread use of drone-based compact systems operated under GPS control. Using a high repetition rate and fast scanning, powerful height imaging is readily achieved from the point swarm recorded. Terrain topography and canopy structures can be assessed and direct provide important information on terrain features, growth status etc, aspects of immediate relevance to agriculture. Information on soil erosion, moisture levels, leaf-area-index (LAI) and many other parameters can also be assessed [174–179].

In addition to distance/height measurements, spectroscopy can be added to provide higher information contents in the lidar data. The differential absorption lidar method (DIAL), where pulses with two neighboring wavelengths are intermittently transmitted, can provide information on important atmospheric gases. Then one wavelength is chosen to match a strong absorption line of the gas of interest, while a second one, off-resonant, serves as a reference [173]. Local carbon dioxide contents reflects the efficacy of photosynthesis and can be measured by lidar [180]. Fluorescence spectroscopy is a further technique, which can be combined with lidar. Then, a lidar pulse of UV wavelength will induce fluorescence in a remote target, and by using a gated array detector the received fluorescence can be recorded and analyzed. Chlorophyll gives rise the two clear peaks, around 690 nm and 740 nm, and their intensity ratio bears information on the concentration of chlorophyll. By also analysing blue-green fluorescence, certain stress conditions, due to, e.g. draught can be studied. A review on some experience in vegetation remote spectroscopy and imaging in given in [181], while fluorescence lidar assessment of the fertilization level can be illustrated by experiments on rice [182]. Lidar fluorescence measurements on vegetation using a mobile, pulsed lidar system is illustrated in figure 15(a).

Agricultural pests constitute a serious threat to crops. Again, lidar techniques can be applied to flying insects, and characterize them with regard to number, wing-beat frequency and fluorescence properties [183–185].

Current and future challenges

Clearly, agriculture and food production face significant challenges to make actual conditions match the needs of an increasing population in the presence of global climate change. There will be strong demands on additional information on crops related to, e.g. fertilization level, and stress due to, e.g. drought and insect attacks. The contribution to the field by lidar will rely on the availability of powerful and cost-efficient systems. As we have noted, drone-based pulsed systems for ground and canopy profiling already have reached a high level of sophistication, but major further improvements are in sight. Data beyond ranging traditionally required complex and heavy pulsed systems. A new promising development is provided by instead using cheap CW lasers in combination with a compact triangulation detection geometry based on the Scheimpflug principle, which allows sharp focusing along the whole transmitted laser beam [187, 188]. The array detector can be read out at a high rate allowing the registration of also fast wing-beats [186, 189]. Such a lidar system is illustrated in figure 15(b), and data on insects and on raindrops, against which discrimination can be performed using polarization properties, are shown in figure 15(c).

A range-resolving fluorescence lidar system carried by a drone is described in [190], and is illustrated in figure 16 [190]. Here, a two-dimensional detector is employed, where pixels corresponding to increasing range along the laser beam are recorded in one direction, and the full fluorescence spectrum at the corresponding measurement point is recorded in the other direction. Such a system is capable to map out the canopy with individual trees and display the fluorescence spectrum with high spatial resolution. This is achieved by using multiple flight passes under GPS control to generate a three-dimensional image, where color coding can display selected fluorescence features.

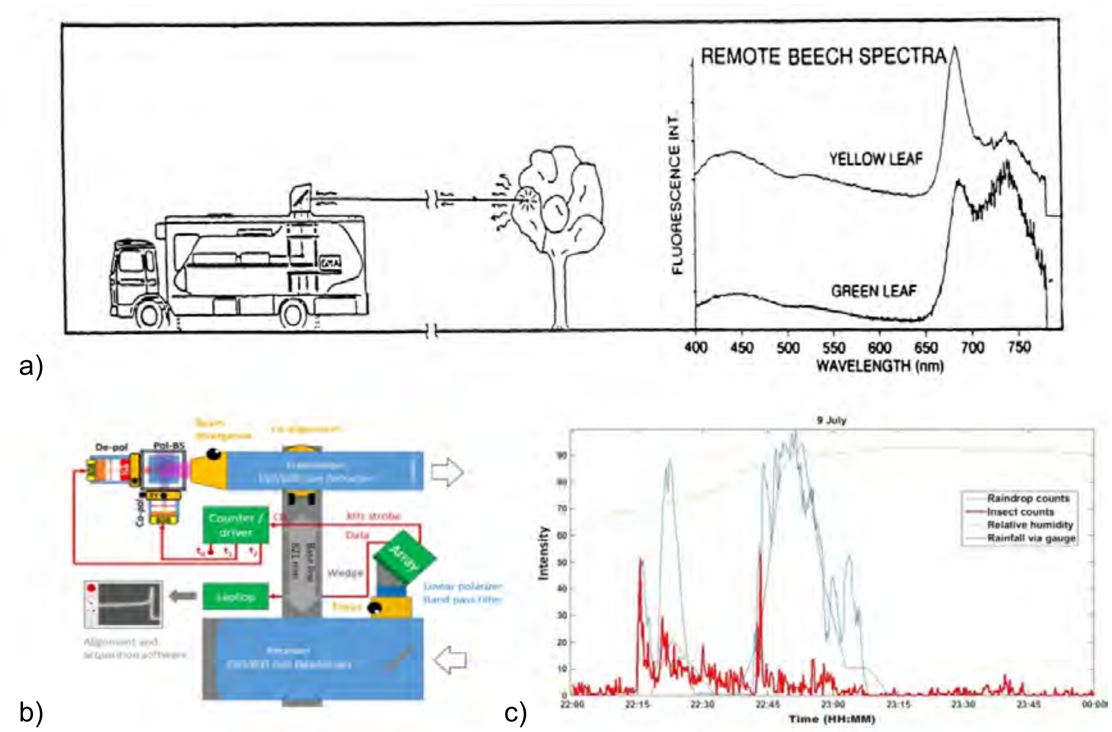

Figure 15. (a) Mobile fluorescence lidar system transmitting UV laser pulses, which induce fluorescence in distant vegetation. Two recorded fluorescence spectra illustrate the difference between leaves with high and low chlorophyll contents. Reproduced from [181]. (b) CW Scheimpflug lidar system equipped with two lasers, which intermittently transmit light with perpendicularly oriented linear polarization. (c) Insects and raindrop signals distinguished by differences in light depolarization, as recorded using a system of the type shown in b). It can be seen how insects are driven down from higher heights into the laser beam at the onset of rainfall. Reproduced from [186].

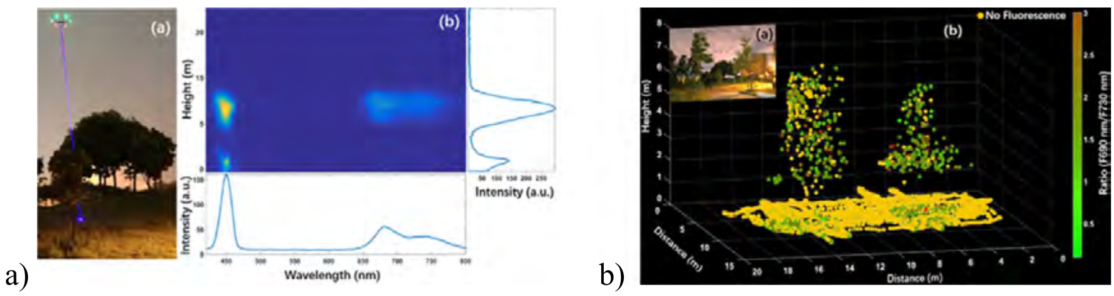

Figure 16. (a) Drone-based multi-spectral lidar system providing range-resolved fluorescence spectra. (b) Data of the kind shown in (a) recorded along multiple drone flight-lines controlled by GPS. Two trees are imaged in false color, mapping the ratio between the two near-IR chlorophyll fluorescence peaks. Reproduced from [190], with permission from Springer Nature.

Elastic backscattering or laser-induced fluorescence (LIF) can be pursued with low-cost multi-mode semiconductor lasers, which are readily available at power level up to several watts. By instead using a narrow-band single-mode laser, which can be tuned to a specific absorption line of an atmospheric constituent, it is possible to map out the concentration of that gas. While water vapor mapping is much needed for improved weather forecasting, the details of the carbon dioxide distribution is of particular interesting in the agricultural sector. Such monitoring using a Scheimpflug system was recently demonstrated [191].

Lidar can also have important applications in horticulture. Short-range fluorescence assessment of maturation status of fruits has been demonstrated [192], and could help in determine optimum harvest time.

Advances in science and technology to meet challenges

Lidar techniques can be expected to have a major impact in precision farming, but clearly many challenges have to be addressed. Widespread application will certainly rely on effective sensors being available at affordable price. Here, the new Scheimpflug lidar concept, both in its elastic (one color) and inelastic (multi-color) variety may be of particular importance. Such systems can be made quite compact and thus be adapted to drone deployment. Generally speaking, drones will become increasingly important in agriculture. The development of the most straight-forward application, ranging, towards ever better performance is benefitting from the tremendous expansion of lidar use in vehicle autonomous driving. Fast lateral scanning also in active, multi-spectral drone-based 3D-lidar systems would constitute a natural but challenging development.

The achievement of full eye safety even in unsupervised systems will become feasible following the future availability of high-power, UV semiconductor lasers.

The demand for ever increasing productivity in agriculture and keeping prices reasonable has led to a strong increase in the use of pesticides, which is a worrying development both in terms of environmental pollution and loss of biodiversity. Powerful monitoring of flying pests would help keep control of invasions, with counter measures reduced to the required minimum. It could also help biological farming to increase its competitiveness.

At the same time as the hard-ware is developing, it is equally important to ensure that software, which produces pedagogical and intuitive representations of the complex raw data is implemented.

It is a disturbing fact that a high percentage of crops, and in particular of fruits, is wasted due to inadequate storage. Foods are frequently stored in a modified atmosphere to increase shelf-life, and the correct operation of packaging machines must be ascertained. Also, it is well known that foods can also be in perfect shape after the printed 'best-before' date has passed. Laser spectroscopy can be used to non-intrusively perform gas analysis of food packages [173]. While now available for packaging machines, a natural development would be a short-range lidar handheld sensor for the customer. Combined with reflectance and fluorescence capability, further powerful assessment of the actual food status could become available. The integration in future smart-phones may become a reality.

Concluding remarks

Optics and photonics have had a major impact on most sectors of human activities, and their impact does not seem to diminish. Climate, environmental and health issues are receiving an ever increasing interest from individuals and authorities alike, and in many cases approaches based on light as a potent information carrier are utilized. Active techniques, utilizing an artificial light source as compared to passive ones (utilizing ambient radiation) are generally more potent but also more expensive. Lidar monitoring of targets (including in the agro-food sector) can be performed from very large to very short ranges, corresponding to satellite-born or hand-held sensors. Lidars of different level of complexity/capability are already influencing the agro-food sector substantially, but current trends indicate the possibility of an increasing impact. Miniaturization and cost effectiveness based on drones and CW laser sources, to complement pulsed ones, will be important.

Acknowledgments

The author gratefully acknowledges the fruitful collaboration with colleagues and students in the agro-food sector, and the financial support from many agencies.

10. Digitization and digital twins in agriculture

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Status
Digitization in agriculture is currently taking place at all steps within a food commodity chain [193, 194], namely:

- the production of agricultural inputs, including fertilizers, pesticides and plant breeding,
- the farming process, including irrigation and crop growing (precision-agriculture equipment, robotics, farm management platforms and agronomy advice and information)
- the trade of raw agricultural produce;
- food processing, where raw agricultural products are manufactured into finished food products,
- food packaging; transport and storage;
- food retail and consumption, which includes both supermarkets and smaller independent traders selling their goods directly to end consumers.

At the farming level digitation is based on the use of IoT [195], big data analysis, as well as AI [196, 197]. At the food processing level, the main trend in emerging digital technologies involves automation or robotics, such as optical systems that automatically sort fruits and vegetables [198], and IoT technologies such as collaborative robots that communicate with one another. Some companies are also experimenting in smart packaging and food printing [199]. In food transportation, different types of sensors (mainly spectroscopic) and analytics allow for greater control over the conditions of the food transportation and storage in order to monitor the freshness, increase the safety and avoid losses through spoiling [200].

Digitization is creating a platform for introducing into agriculture the concept of DTs, which have been widely adopted in other disciplines. DT, according to Clark's definition is '*a dynamic virtual representation of a physical object or system, usually across multiple stages of its lifecycle, that uses real-world data, simulation, or ML models combined with data analysis to enable understanding, learning, and reasoning*' [201]. In general the benefits of DT applications include reduced production times and costs, hiding the complexity of integrating heterogeneous technologies, creating safer working environments and establishing more environmentally sustainable operations. DTs in agriculture involve the creation of virtual models that mimic the characteristics and behavior of physical farms. The architectural framework for implementing DTs in agriculture, as proposed by Peladarinos *et al* in [121], is shown in figure 17.

It highlights the key components and interactions of DTs in agriculture, showcasing their role in data collection, preprocessing, modeling, simulation, analytics, decision support, visualization, and control, ultimately aiding in optimizing farm operations and improving decision-making processes. The DTs' models are built using a combination of data from various sources, including sensors, drones, satellites, and historical records. By continuously collecting and analysing data, DTs provide farmers with valuable insights into crop health, soil conditions, weather patterns, and resource utilization. The interconnections between all components play the vital role as they are essential for functioning of the DT system in integrating manner. More details on the possible frameworks for implementation of DTs in agriculture are given in [121, 202–204].

Despite to these benefits DT are presently not widely utilized in agricultural applications as shown in the literature reviews published by the groups from the Wageningen University [205, 206] and TU Wien [207]. The published research in Agricultural DTs in the period from 2017 (the first paper [208]) up to 2022 can be classified within the following applications and use cases [207]:

Crops: monitoring, resource optimization and cultivation support. This is the most frequent category with the most common usage of photonics sensors for data collection. The representative examples include:

- a multi-agent approach to create a crop DT by monitoring growth and predicting outcomes through simulation [202] as well as detect anomalous states and recommend appropriate measures for correction [203];

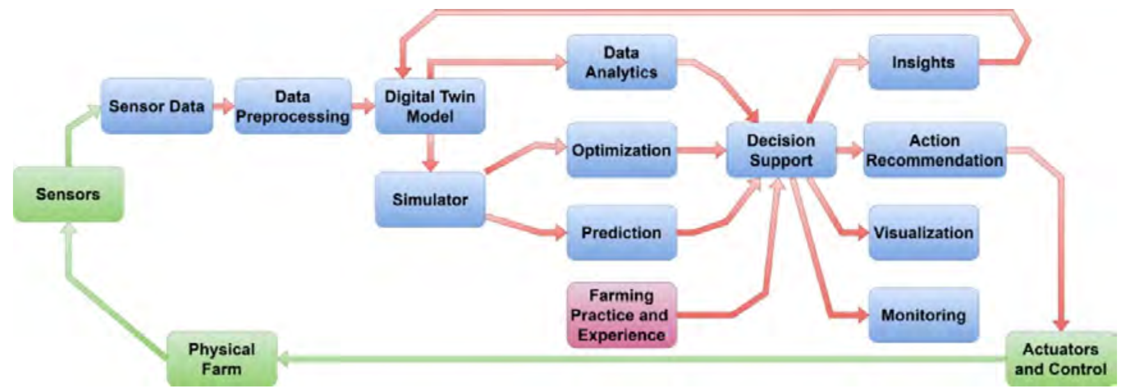

Figure 17. The architectural framework for implementing DTs in agriculture. Reproduced from [121]. CC BY 4.0.

- an orchard DT; using 3D lidar and cameras a DT of each tree is created and updated with the goal to provide real-time conditions monitoring and decision support on a large number of trees and reducing the farmers labor requirements [209];
- a farmland DT for plant monitoring and decision making support based on low-powered IoT wireless sensor network and drone imagery [204];
- crop irrigation optimization for yield improvement based on IoT based DT using both localized (sensor on site) and remote sensing methods [210];
- a smart service for potato harvesters by the creation of a 'Digital (twin of a) potato', which allows manufacturers and farmers to minimize damage of potatoes and ensure optimal calibration of a potato harvester [211].

Livestock: Monitoring, management and optimization. The representative examples include [212]:

- DT of a pig farm to monitor pig health status and prevent diseases through controlling the animals parameters and the working conditions of a farm;
- DT of a cow to predict heat, estruses and health according to their behavior,
- DT of bee colonies based on GPS tracking system along with humidity, temperature and weight sensors.

Urban, controlled environment and aquaponic farms. The representative examples include:

- vertical planting IoT-based DT with focus on sensing and controlling the conditions via light and misting [212];
- DT of a soft-shell crab farming based on low cost IoT network with focus on real-time water quality monitoring [208];
- DT for general application within commercial greenhouses with focus on optimization of energy consumption and management [213].

The other applications and use cases in agriculture refers also to such areas as environmental transparency, machinery management (similar to industrial solutions) and improving of meat and fruit value chain [207].

Current and future challenges

While DTs in general hold immense potential, in agriculture there are several additional challenges that need to be addressed. The most significant challenge refers to those operations which have to do with living subjects, like animals and plants or perishable products. While DTs are ideal to provide insights into such complex systems, their integration with the physical twin can be difficult. Also the open questions include how model fidelity regarding biological systems can be evaluated and what methods can be leveraged for facilitating interactions between Physical and DTs. In agriculture, human-made systems like agricultural equipment could be easier to synchronize with the virtual system, unlike natural systems like animals or land parcels. The second challenge lies in the spatio-temporal dimension of DTs in agriculture, which range from an individual plant (or even its part such as a root or a leaf) to twins of land parcels, farms, or regions [205]. Therefore it is necessary to introduce a variety of instruments for data collection and consider effects across these scales. On the temporal dimension, agricultural DTs differ due to the slower response rates of their physical twins. Agricultural processes like growing of plants tend to evolve relatively slow, so at least initially there is no need for high-frequency interactions between physical and DTs. On the other hand, methods to reconcile data with significant temporal differences will be required, in-order to take full advantage of available data sources and provide context to entity behavior at different temporal-scales.

Another ongoing issue is data quality and pre-processing. Without good data, models will inevitably under-perform. Improvements in outlier detection, data generation and integration of diverse data sources as well as scenarios for ensuring data accuracy and reliability are needed. These issues are linked with the need of standardization at different levels of architectural framework (figure 17). In future, in a fully connected and interactive world, different physical assets will be interacting with each other and the corresponding DTs also have to do so. In order to facilitate these interactions there is a need for standards cutting across different domain areas. These standards can range from hardware (IoT sensors, their networks) to the file format of the data storage, data compression and the data protection requirements addressing differences in the laws when spread over different geographical areas and disciplines. Obviously, there is also a need for standardized protocols and frameworks to enable interoperability between different DT platforms [207].

Another aspect affecting the adoption of DTs in agriculture is that the community has to build trust in the interplay of the DT components for its correctness. This trust is essential to create DTs that can accurately represent the inner workings of a system, propose maintenance strategies and alternative ways of management. Yet, building this trust in agriculture is difficult, because many decisions affect living systems where, unlike in other disciplines, consequences can be hard to reverse [196, 214].

Last but not least, the frequent lack of data culture in agriculture and the cost of implementing and maintaining DT systems, including sensors' networks and other data collection means, can become a barrier for small-scale farmers, as well as one of the sources of friction between big and small agriculture producers [194, 214].

Advances in science and technology to meet challenges

To address the first challenge, a big variety of new, low cost sensors are under development [195, 215] the design and technology of sensors with extended spectral, resolution and precision capabilities are already present in research labs and are step by step transferred to industry. The main directions in photonics sensors in agro-food applications, as shown in this paper, are focused on extension of the applied wavelengths ranging from UV through visible, MIR up to THz. Having this in mind, implementation of a variety of spectroscopic methods (FTIR, fluorescence, Raman) into miniaturized sensors by means of photonics integrated circuits, fiber optics, Lab-on Chip, MEMS/MOEMS equipped with multiplicity of functionalities is on its way.

Other technologies generating the highest interest within agriculture right now are unmanned aerial systems (UAS), fitted with visible, IR, or/and hyperspectral cameras and other imaging sensors (e.g. LIDARs). The improved versions of the existing sensors are able to consistently and quickly collect higher-resolution RGB images over increasingly larger areas, being both ruggedized, with low power consumption and inexpensive (UAVs frequently crash) [204]. Current improvements of detectors' spatio-temporal capabilities of physically larger sensors, such as better resolution and faster shutter speeds, already allow higher and faster UAS flights for PA.

Current research European projects include the DT development for individual crops and their individual biophysiological environment, as can be seen at the University of Natural Resources and Live Sciences [207] and at the University of Wageningen [121, 205]. These examples involve also successful implementation of ML and deep learning techniques. Moreover, it was shown that AI significantly processes IoT data through continuously enhanced algorithms that leverage updated user data. Leveraging and fusing/integrating such time-series data, a user's DT has the potential to suggest actions for controlling or mitigating potentially hazardous situations regarding crop health and productivity, or even failures of safety mechanisms of farm machinery, plant production equipment, post-harvest transportation or storage equipment situations in which DTs may visualize alarm signals to stakeholders.

On the other hand, with progressing digitization and development of DTs there are significant efforts to build entire agriculture ecosystem. The notion of`farm to plate' involves several entities which work in tandem to provide quality food to the end consumer in a just-in time environment. With IoT technology at each stage of the supply chain, it introduces potential cybersecurity threats since a security breach in just-in-time distribution system could also have a serious cascading effects on the entire supply chain. For this reasons the important works related to cybersecurity in the domain are in progress [216]. This in turn, together with increasing precision and reliability of sensors and algorithms, build the trust among users' community [194, 196].

Concluding remarks

Climate change and increase in the world population are the chief drivers for technology in agriculture. Automation motivated by digital revolution, sensing technologies, 5G, and agricultural robots and aerial systems equipped with 2D/3D machine vision accompanied by resource optimization must be adopted in the agricultural sector in order to influence higher and qualitative crops. DTs have the potential to revolutionize agriculture by optimizing resource utilization, reducing environmental impact, and increasing crop yields. However the close collaboration between technicians, farmers and policy makers is strongly required to drive DT adoption.

As technology advances, DTs role in food production, despite the challenges and unsolved till now problems, will continue to grow. DTs' growth and expansion cannot be imagined without the significant participation of photonics technology in DTs. To successfully develop DT, data capture and delivery through efficient, reliable and low cost sensing and data communication system is evidently necessary. Also the community must become familiar with a variety of related technologies including IoT, AI and big data—most of these technologies are still considered new fields of experimentation in agriculture. Once the community gains confidence around them and adopt best practices for their application, we are likely to see more DTs with innovative photonics solutions emerging in prototype and deployed levels in world agriculture.

Acknowledgment

This work was partly supported by the statutory funds of the Institute of Micromechanics and Photonics, Warsaw University of Technology.

Chapter 2: Spectrometry and spectral sensors

11. Ensuring food for all: state of the art and future trends

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Status

Advances in sensing technologies, including those belonging to vibrational spectroscopy [mid (MIR), near (NIR), RS and HSI], have allowed for the development of innovative applications in a wide range of fields, among others, in agriculture and food sciences [217, 218]. The implementation and utilization of vibrational spectroscopy has been possible by the current improvements in non-destructive analysis, developments in handheld instruments and spectrometer miniaturization [219], the ability of analysing low sample volumes, the advances in chemical and pattern recognition algorithms [220], as well as the implementation of automation and remote analysis including at/in/on-line analysis [221].

The use of vibrational spectroscopy not only allows the non-destructive analysis of samples but also provides with information and knowledge about the entire food supply and value chains, including food manufacturing processes [217, 218]. Nevertheless, the utilization of vibrational spectroscopy encounters different challenges, some of them related to how the information can be extracted from the technological application, and to the evaluation of complex data sets [217, 218, 220].

Traditionally, these techniques have been used to measure or predict the chemical composition of different foods (e.g. protein, moisture, starch) instead of relying on cumbersome and time consuming traditional chemical analysis that are unsuitable for evaluating fresh food ingredients and products. Consequently, these techniques have been incorporated as tools into management systems along the food supply and value chains [222] as they are relatively inexpensive, easy to operate, and require little or no sample preparation allowing them to be used in-line or at-line [221].

The utilization of vibrational spectroscopy has been associated with assuring and monitoring food safety to protect consumers from the increased number of issues associated with food security (e.g. fraud, contamination), which are linked with mortality, human distress, wellbeing, and economic burden (figure 18) [223]. In this context, vibrational spectroscopy provides useful information to make informed decisions about the safety of specific foods and food ingredients [222]. These techniques have also been of fundamental importance in the digital economy and the fourth revolution [218].

Current and future challenges

It is well accepted that vibrational spectroscopy techniques have clear advantages over traditional analytical methods, as these methods can be objective, cost effective and provide rapid, reproducible results, with continuous operation [217, 218, 224]. Public health and consumer safety authorities are demanding the development of rapid screening techniques that can be used beyond the laboratory, such as in the field, manufacturing plants, supermarkets and even at home, to evaluate not only the composition and quality of foods but also to guarantee their safety [217, 218, 224]. Although vibrational spectroscopy has been proven to be of importance along the food supply and value chains, the adoption of these technologies has been slow due to different factors. For example, accessibility to instrumentation due to its cost has been one of the main factors limiting its utilization, as defined by the different stakeholders in the food sector. Other factors, such as the skills available to implement and fully exploit the use of vibrational spectroscopy, are constrained by the lack of instructors and teaching resources to deliver appropriate training. There is a need for training, not only of researchers, but also for different stakeholders including managers and consumers. Challenges associated with assuring confidence in the use of the different vibrational spectroscopy methods, as well as how to effectively use the data, are still main barriers faced by the food industry. Furthermore, is still not clear for many users how these technologies will contribute to sustainability as well as to preserve the identity of the food processes. The implementation of vibrational spectroscopy-based technologies requires the creation of mathematical models that are developed to quantify different chemical constituents of the sample, to monitor composition, contamination, fraud, etc.

Above challenges are in contrast with the advantages that the utilization of vibrational spectroscopy offers, such as a real-time monitoring throughout the food manufacturing process (e.g. dairy, brewing), specificity, sensitivity, and adaptability to almost all the different aspects in the supply and value chains.

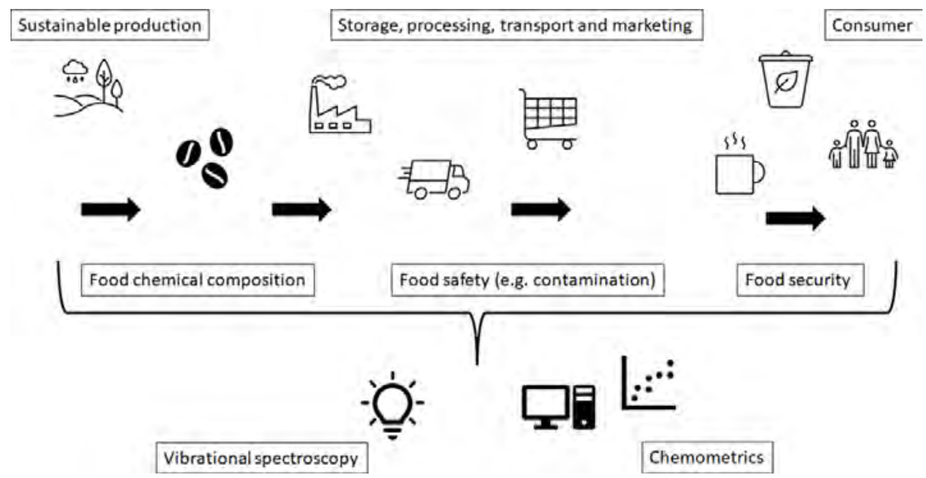

Figure 18. The farm to fork journey of food and food ingredients is monitored using vibrational spectroscopy and chemometrics.

Furthermore, these technologies have demonstrated their contribution as tools in sustainable food systems, contributing to reducing the cost (e.g. less energy, reagents) and time of analysis in the circular economy.

Advances in science and technology to meet challenges

Different advances and developments in the state-of-the-art of vibrational spectroscopy are contributing to the incorporation of these technologies into the food supply and value chains. Some of these advances are discussed in the section below.

Handheld and miniaturization. The miniaturization of spectrometers (NIR and MIR) has evolved through developments in micro-electro-mechanical (MEMS) and micro-opto-electro-mechanical (MOEMS) systems [219]. Handheld and portable spectrometers have been based on different types of detectors (e.g. array detectors, single detector devices) that have contributed to the collection of data using different wavelength ranges (e.g. indium gallium arsenide is the preferred material when manufacturing detectors) [219]. The utilization of single-detector systems has determined the development of alternative and low-cost instruments [219].

HSI. Other important technological advances are those associated with developments in HSI techniques. By combining imaging techniques with vibrational spectroscopy, the sample can be analyzed both spatially and spectroscopically [111, 225]. The incorporation of images has enhanced the ability of vibrational spectroscopy to gain in-depth detailed information about the concentration and distribution of the different compounds or metabolites in the sample's composition [111, 225]. The utilization of HSI in food analysis has boosted our capabilities towards a better understanding of the intricated properties of food [111, 225]. One of the benefits of the use of HSI is the ability to simultaneously collect information on the structural and chemical composition of the analyzed food [111, 225].

New algorithms and pre-processing. Pre-processing is highly important to obtain a balance between the quality of the spectra and the meaningful information available on the food. Pre-processing is required to achieve a trade-off between the data analysis and interpretation, ensuring the accuracy and precision of the final outcomes. Progress in data analytics and chemometrics has contributed to developments in pre-processing techniques where new methods continue to appear, such as multivariate curve resolution (MCR) combined with wrapping, block-scaling and multi-block approaches [220, 226].

Network of instruments. The network of instruments will allow to detect different levels of information offering a holistic analysis of food quality and safety, and consequently of the whole food supply and value chains [227]. The utilization of a network of instruments will contribute to the improvements in the analytical ability and efficiency of the current measurement systems. The use of networking also allows for the evaluation and detection of different and multiple analytes where the integration of different instruments is one of the main advantages. In addition, the increased connectivity has made it possible that the user can remotely access the calibration, minimizing the calibration time. This technology has fostered and increased the communication between food producers, retailers, authorities and consumers, in their decision-making process. Overall, these technologies will enable and improve our understanding of food systems allowing for a better management of natural resources, making food production more sustainable.

Concluding remarks

The routine and commercial implementation of vibrational spectroscopy in the food supply and value chains is in continuous development. Regardless of the advances in technology and instrumentation, the implementation of vibrational spectroscopy requires the incorporation of data mining and ML tools. Although, for some users, the utilization of vibrational spectroscopy is still described as a 'black box' approach.

In addition, the skills available to implement and fully exploit the use of vibrational spectroscopy are constrained by the lack of instructors and teaching resources, hampering to deliver appropriate training. There is a need for training, not only of researchers, but also for the users and ultimately the consumers.

A highlight on the use of vibrational spectroscopy is that it fosters the integration of knowledge from many research fields (e.g. spectroscopy, analytical chemistry, data analytics, biology, biochemistry and chemistry). This key characteristic has determined the unique multidisciplinary nature of vibrational spectroscopy in food sciences. Preserving the multidisciplinary approach is critical for further development and implementation of these technologies, moving from the black box approach to a robust analytical method. These techniques are allowing for novel solutions that will challenge the way food is analyzed, as well as increase the efficiency, sustainability, flexibility, agility, and resilience of the food supply and value chains, from the farmer to the consumer (e.g. fork to farm approach).

Acknowledgment

The support of the University of Queensland is acknowledged.

12. NIR spectral sensors to ensure the integrity along the entire food chain

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Status

Product and process control, authentication and monitoring are key issues for the food industry, affecting its efficiency, trademark image, economic performance, and sustainability. The increasing complexity of the food supply chains has created more opportunities for food fraud, resulting in many food crises over the years, which have reduced consumer confidence in the industry, inspection bodies and policy makers. This situation has led to an increased focus on developing measures to ensure the food integrity throughout the entire food chain, 'from farm to fork'. To verify the integrity of food products it has been necessary to update the current analytical and sampling control systems, through the development of modern and cost-effective analytical methods. Recent developments in NIRS and advances in big data analytics offer new opportunities to provide solutions to the industry in this challenging area.

Near-infrared (NIR) technology is defined as a vibrational spectroscopic technique, based on the absorption produced when near infrared radiation ↓ between 780 nm and 2500 nm ↓ vibrates at the same specific frequency as the molecular bonds of the product being analyzed [228, 229]. NIR spectroscopy was developed as an analytical technique in the late 1960s by Karl Norris working on agricultural applications, while the first commercially available instrument appeared in the early 1970s [230]. Since then, NIRS technology has evolved enormously and has become increasingly widespread and accepted because it enables non-destructive, rapid, accurate, cost-effective and environmentally friendly analysis of a wide range of food products as well as the determination of numerous chemical-physical and even sensory properties of these products. In addition, this technology provides a sustainable digital signal, which enables NIRS to be used as an IoT device [231, 232], allowing the interconnectivity and interoperability with other signals and other information and communication technologies (ITCs). This last aspect is essential in the current global and food industry situation, where everything is digitalized and connected, now living the transition between Industry 4.0 and 5.0.

In the early days of NIRS, the applications were developed using benchtop instruments operating under controlled laboratory environments. However, over the last few decades, the important advances in the design and construction of a new generation of miniaturized and highly portable NIRS instruments [233] have opened up many new possibilities for the on-site, in-line and on-line use of NIR sensors, which can now be used along the food chain, enabling real-time decision making in the field. Importantly, some of the new applications were unthinkable just a few years ago (such as the analysis of *in vivo* animals, in-field measurements of crops and trees or on-line process control), making food control systems now more robust, intelligent, massive, interoperable, and accessible [234–239]. Figure 19 shows some examples of these applications made possible by recent advances in instrumentation. In (a), the spectral analysis of spinach plants in the field using a portable instrument is shown, carried out to determine their dry matter, soluble solids and nitrate content, facilitating decisions on optimal fertilization strategies, harvesting time and industrial destination. In (b), an analysis of live hens is shown to measure their abdominal fat, allowing on-farm decisions to be made on their photo stimulation and laying induction. This analysis was carried out with an ultra-compact and very low-cost spectrometer, essential characteristics for its final implementation in the industry. Image (c) illustrates the on-line analysis of tenderloins, applied to determine their chemical composition, to authenticate the breed of the animal and determine whether the meat has been previously frozen or not, as key aspects of the quality, safety and traceability of meat products. Finally, (d) the use of a very low-cost portable NIRS sensor suitable for the analysis of olive oils in transmission mode using disposable vials is presented. This example focuses on the determination of quality parameters (acidity, waxes, esters, fatty acid profile, polyphenols or sensory profile) and commercial classification of the product, thus providing industrialists with an affordable analysis methodology for self-control in olive oil mills and to provide consumers with more detailed information on a high-value food product.

Current and future challenges

As mentioned above, the use of NIRS sensors at different stages of the food production and supply chain is currently gaining particular importance as an integral and essential technology for food traceability, quality, and safety assurance. Although significant progress has been made during this century, it should be

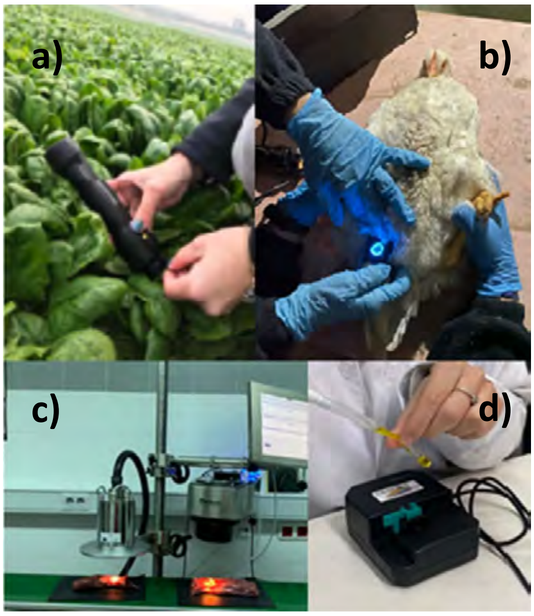

Figure 19. *In-situ* measurements using the portable NIR instruments.

emphasized that many challenges remain to can exploit the full analytical potential of NIRS for food integrity assessment. The complex nature of food poses significant challenges to the application of NIRS, requiring the development of specific and product-dedicated databases for each type of product, sophisticated mathematical data processing or special considerations regarding sampling and population variability. The main challenges and opportunities of NIRS as an intelligent sensing device are:

- Improvement of on-site analysis, based on new instrumentation or data processing technologies, also enabling new applications. Although NIR sensors are extremely well suited for portable or hand-held use, their potential has only relatively recently been recognized at the research level, and in many cases specific developments and adaptations are still needed before they can be adopted by the food sector. Moreover, the industry needs to understand the benefits and opportunities that this technology can offer before decisions can be made about its deployment.
- The high heterogeneity of agri-food products requires improved sampling to increase the amount of product inspected and reduce the associated risks. The role of NIRS for the massive sampling of bulk products and production batches should be further explored, highlighting one of its main advantages—not fully exploited—which is the possibility of reducing the sampling error and therefore the overall analytical error, by having a more precise response.
- Integration and combination of the NIR signal with other sensors that can provide complementary information, to solve complex issues that cannot be solved with a single sensor.
- The development of NIRS as a non-targeted method, spreading the potential of using the NIR spectrum as a product fingerprint that can provide information on its quality, safety and authenticity, and be essential for process control. This approach is based on exploiting the full potential of NIRS sensors, without the need to train them with other analytical reference methods [240, 241].
- Improve scientific knowledge of methods for establishing, maintaining, and transferring robust calibrations suitable for industrial and commercial use. For this technology to work in the food industry, robust and accurate models are needed that are also reproducible across a network of instruments. In addition, the management and interpretation of the huge amount of data generated by NIR sensors working on-line in continuous operation may require the use of more sophisticated mathematical data processing methods, such as ML and AI.

Advances in science and technology to meet challenges

The incorporation and adoption of NIRS technology by the food sector as an integral analytical technology to solve food integrity issues is being demanded by more and more companies every day. In order to successfully transfer the knowledge developed at the research level to the commercial and industrial level, intensive research is being carried out to address the aforementioned challenges associated with the use of NIR spectral sensors throughout the food supply chain.

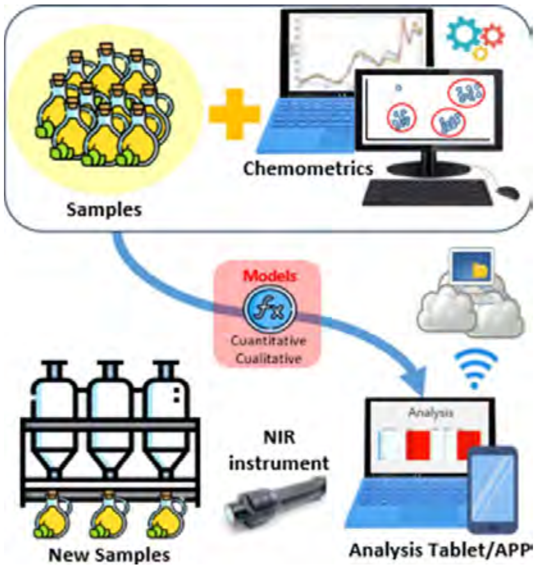

Figure 20. NIRS analysis integrated in a support decision platform.

One of the most significant and notable advances, as already mentioned, has been the improvement in instrumentation. However, real-time monitoring throughout the food chain can still be limited by equipment limitations and data transmission issues. The development of more sensitive, portable, robust and versatile NIR sensors is crucial to obtaining accurate and reliable data. Today, a wide variety of NIRS sensors with different optical designs and characteristics tailored for different applications are being introduced to the market. A notable trend is the miniaturization of these sensors, using technologies such as linear variable filters (LVFs), Fourier transform (FT) or MEMSs [242], making them more portable and accessible, and enabling on-site analysis, eliminating the need to transport samples to the laboratory. Furthermore, the development of low-cost and user-friendly NIRS software will make it accessible to a wider range of users and companies, in particular SMEs (small and medium-sized enterprises), for whom cheaper technologies are key to access and successful implementation in their production processes.

The role of HSI, including the spatial to spectral dimension, is clear when combining different sensors to obtain more information. HSI can make measurements in different ways and regions of the electromagnetic spectrum (NIR reflectance, Raman, fluorescence and thermal spectral regions), increasing the potential for inspection. The combination of several spectral signals in the same instrument is still under development, with some prototypes appearing, such as the multi-mode handheld instrument combining visible, NIR and fluorescence [243]. These instruments result in a more complex signal, which would imply the need for advances in calibration techniques and chemometrics to extract the valuable information to obtain robust predictive models. The integration of data analytics and ML or AI enables real-time analysis, anomaly detection and prediction of potential problems in food products, thus improving overall quality control.

In addition, new approaches to data processing based on the development of compliance tests, the definition of standards and deviations, and the use of spectral information to design early warning systems provide additional benefits and business cases for implementing NIRS as a non-targeted method.

Finally, another key aspect related to spectral sensors and application development is that the systems have a user-friendly interface that provides only the necessary information to the final user, and can be integrated into the industry dashboard to facilitate automated decision making. In this regard, NIRS companies focus on ease of use and user interface, making them more accessible to a wide range of users and applications. In addition, the combination of the NIRS signal with ITCs, including IoT platforms, has facilitated remote monitoring and data sharing (figure 20). This connectivity enables the development of a more efficient and transparent platform, both for the producer to self-monitor the process and to provide more detailed information to consumers through more comprehensive digital labeling of food products.

Concluding remarks

NIR spectroscopy, coupled with chemometrics and, more recently, the combination of NIR data with ITCs and other sensor signals, could play a crucial role in the development of intelligent systems for in-situ food quality control and authentication. Although this technology has made significant progress in recent years, a number of issues and challenges remain to be addressed, mainly related to instrumentation improvement, data processing and sensor integration and interoperability. Furthermore, exploring the use of NIRS to treat any non-compliant product, both for process control and fraud detection purposes, based solely on spectral information, could undoubtedly revolutionize the assessment of food integrity and the design of modern control systems at an industrial level. In the future, new advances in science and technology, combined with AI strategies (algorithms, DTs…), will lead to increased accuracy, versatility and accessibility, consolidating NIR spectroscopy as an invaluable tool in a wide range of applications. These advances will contribute to improved quality control, safety and efficiency in various industries.

NIRS, coupled with chemometrics and, more recently, the combination of NIR data with ITCs and other sensor signals, could play a crucial role in the development of smart systems for in-situ food quality control and authentication. Although this technology has made significant progress in recent years, a number of issues and challenges remain to be addressed, mainly related to instrument improvement, data processing and sensor integration and interoperability. Furthermore, exploring the use of NIRS to treat any non-compliant product, both for process control and fraud detection purposes, based solely on spectral information, could undoubtedly revolutionize the assessment of food integrity and the design of modern control systems at an industrial level. In the future, new advances in science and technology, combined with AI strategies (algorithms, DTs…), will lead to increase accuracy, versatility, and accessibility, consolidating NIR spectroscopy as an extreme valuable tool in a wide range of applications. These advances will contribute to improved quality control, enhanced safety, and greater efficiency across various industries.

Acknowledgments

This contribution to the Roadmap has been developed under the projects ‘NIRS technology and IoT platforms form for ensuring the integrity of high added value Spanish products: Iberian cured ham and extra-virgin olive oil’ (PID2019-111387RB-I00), NIROLEO: Innovation in olive oil quality control in olive mills through the use of NIRS sensors (GOPO-CO-20-0002) and the COST Action ‘European Network for assuring food integrity using non-destructive spectral sensors’ (SensorFINT, CA19145).

13. Application of near infrared spectroscopy in the analysis of cultivated mushrooms

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Status

For thousands of years, people have used edible mushrooms as a tasty food and a vital source of nutrition (figure 21). The biological value of mushroom proteins, their polysaccharide and trace element content, and their specific endogenous antioxidant property play important role in nutrition. The main components of secondary metabolites specific to mushrooms are phenols, phenolic acids, tannins, lignans, terpenoids and flavonoids. They are valuable source of vitamin D, riboflavin, niacin, pantothenic acid, ergothioneine [244]. They have a wide range of physiological effects: stimulate metabolism, reduce serum cholesterol levels due to their polyunsaturated fatty acid content, and regulate blood sugar levels. Many beneficial effects are attributed to mushrooms in enzyme induction, anti-tumor cell action, and in defense against oxidative stress damage [245, 246]. Mushrooms are regarded as a great source of protein in addition to being low in calories. Although plants typically lack the amino acid composition needed by the human body [247], the proteins found in mushrooms and animals have comparable amino acid compositions, although their ratios differ [248].

The global market for mushrooms was worth USD 50.3 billion in 2021, but it is expected to grow by 9.7% annually between 2022 and 2030 due to increased consumer demand. The growth of the vegan population worldwide, requiring a protein-rich diet, is expected to be a major driver of the market over the period forecasted [249].

The Food and Agriculture Organization (FAO) and the World Health Organization (WHO) now suggest mushrooms as 'super foods,' and consumers like them because of their high nutritional content [250].

Expectations of quality and, by extension, of the analytical techniques employed in quality control are changing as a result of increased consumer demand. The need to create quick, dependable, eco-friendly, and non-destructive imaging and spectroscopic methods based on NIR light has consequently grown.

Current and future challenges

The conditions of development, harvest, and storage all affect the color, shape, size, flavor, nutritional value, microbial spoiling, and enzymatic or chemical deterioration of mushrooms. Even before harvest, ongoing quality monitoring is required since the biochemical processes of decomposition and degradation cannot be foreseen. For this, NIR techniques (HSI or Spectroscopy—NIR) are used.

Whole mushrooms can have surface damage detected using HSI. Principal component analysis (PCA) was applied to the hyper-cubes through score image analysis to provide an unsupervised classification method for impact damage diagnosis. It is clear that the HSI method is most likely to highlight the distinctions between tissue that is healthy and tissue that is damaged. The discolored samples might have an overall classification accuracy (OCA) of more than 79% when PCA is applied to the spectral data. Mushrooms exposed to freezing were identified using HSI before the telltale symptoms of freeze-damage, such as browning and shrinkage, became apparent [251]. For this, linear discriminant analysis (LDA), a supervised classification algorithm, was employed. In order to detect brown blotching and enzymatic browning of mushrooms with OCA ranging from 69.4%–95%–100%, chemometric evaluation of HSI data was conducted using PLSs discriminant analysis (PLS-DA). An OCA ranging from 92.84 to 94.19% was attained for mechanical damage identification using support vector machines (SVMs) and artificial neural networks (ANNs). Due to their high water content (more than 90%) and vitamin content, mushrooms are among the most susceptible agricultural products to deterioration. In summary, figuring out the moisture content of mushrooms is a critical matter. Using the obtained hyperspectral data, PLS ($R^2 = 0.89$) or MLR and PCR models were developed and effectively used to predict the moisture content of the whole mushroom [251, 252].

Numerous attributes can be quantitatively predicted using analytical approaches based on NIR radiation in conjunction with other chemometric methodologies. Examples include the moisture content [253] which is important for shelf life and freshness, the protein content [254], which is mainly composed of essential amino acids and is mainly responsible for the nutritional value, and the polysaccharide content [255].

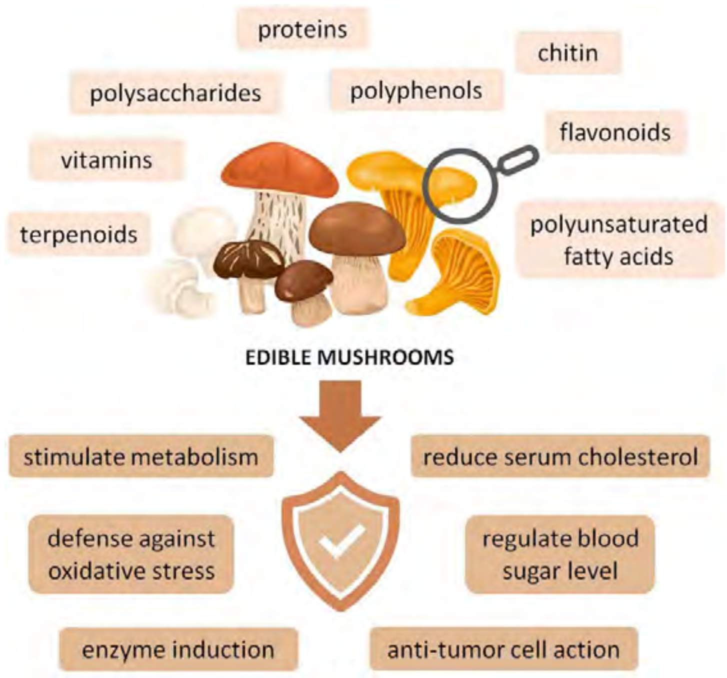

Figure 21. The valuable properties and effects of mushrooms.

Zaukuu *et al* [256] have provided a thorough summary of the fundamentals of molecular spectroscopy techniques, such as HSI and NIR, and how they can be used to identify and adulterate mushrooms.

Advances in science and technology to meet challenges

Since the genetic traits of the strains are what mostly define quality in the case of mushrooms, breeding the correct individuals and choosing strains with superior traits are both crucial to the cultivation's success [257]. Unlike cultivated plants that have been grown for generations, the gene pool from which the mushroom can be bred is quite small, giving the breeders a limited base from which to work. Most of the mushroom varieties that are grown today can be traced back to an old breeding variety of oyster and agaricus mushroom hybrids. In addition, intensively cultivated mushroom species, do not have 'gene centres' unlike in the case of plants [258].

In cultivation, there is a huge variability in color, morphology, spore formation, texture, etc… From a taxonomic point of view, this variability poses a challenge in species identification. Due to the difficulties in identifying taxonomic groups, breeders and researchers are often faced with misunderstandings and may encounter difficulties. These challenges include, for example, selecting the right environmental parameters or breeding new strains with good production potential based on the researchers' identification of the variety. For all the above reasons, variety identification is the most important step when it comes to avoiding taxonomic confusion and improve genetic traits [259]. Classification of cultivated mushroom samples is also of key importance regarding the possibility of geographical origin and variety identification [260].

On the one hand, to distinguish edible and non-edible mushrooms, and on the other hand, to detect fraud resulting from the mixing of excellent-, poor quality mushrooms for economic gain are an important objective. Mushrooms contain secondary metabolites, such as polyphenols, which can determine the chemical composition depending on the geographical region, species, and growth conditions, and can help in identifying the origin. These secondary metabolites play a protective role in the survival of the mushroom under various stress conditions and pathogen attacks. Their production and accumulation are related also to light, water and temperature [261].

To satisfy rising consumer demand, it is critical to create cultivars with ever higher nutritional values in addition to geographic and varietal identification. The creation of novel cultivar candidates offers the chance to create a variety with better enzyme activity and favorable free amino acid concentration [262].

The aforementioned examples have significantly increased the demand for analytical techniques to assess the quantity, quality and authenticity of food ingredients. As a result, there is a continuous increase in the design and development of non-destructive, quick, accurate, portable, and/or hand-held HSI and NIR

Figure 22. Possibilities for non-destructive analysis using near infrared radiation.

instruments. NIR equipment have become widely used in agriculture due to their rapid development (figure 22) [263]

Concluding remarks

Growing consumer awareness over the past decade, has prompted food scientists to create new techniques for quality management and monitoring. When it comes to creating innovative methods, efficiency and environmental friendliness are crucial. For both farmers and dealers, keeping an eye on the quality of mushrooms is essential because of their high water content, quick respiration rate, unique surface structure, and therefore quick aging process after harvest. Freshness is frequently monitored using conventional techniques such sensory analysis, enzyme activity assays, and color and texture determination. Food safety and quality depend on the classification and identification of mushrooms, including species, varieties, and place of origin.

These tests, however, are often time-consuming and involve techniques that destroy the sample. To distinguish and evaluate mushrooms, modern analytical methods like HSI and NIR are frequently employed.

For the scientific analysis of the multidimensional data present in various analytical methods, chemometrics is an effective tool. Furthermore, a thorough assessment of its chemical makeup and concentration can aid in our comprehension of the nutritional qualities of mushrooms.

Acknowledgment

We are grateful for the support of Doctoral School of Food Science of the Hungarian University of Agricultural and Life Sciences

14. Fruit quality control by mid-infrared multi-species trace gas sensing

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Status

A continuous supply of fruits and vegetables throughout the year requires long-term large-scale storage. Fruits are usually stored under low oxygen and high carbon dioxide conditions to maximize their shelf life. Lack of proper storage facilities and infrastructure can lead to significant loss of the stored products, up to 10% for various geographical locations [264]. It is therefore a challenge to preserve the quality of agro-products during long-term storage.

One effective way to reduce losses in commercial-scale storage is to control adaptively and dynamically the storage atmosphere based on certain stress indicators. The current inability to undertake timely and effective actions leads to serious losses that could be prevented if continuous quality monitoring of stored products were possible. Additional information on damage, rotting and ripening stages could further help to determine the optimal moment to sell stored fresh food products. Storage facilities would thus strongly benefit from new methods that could improve the monitoring of these products.

To obtain a deeper insight into the physiological and pathological status, various volatile compounds released by fruits are considered extremely relevant, such as ethylene as ripening indicator [265], ethanol, acetaldehyde and ethylacetate as markers for fermentation [266], methanol and acetone as rotting indicators [267] and ethane as chilling injury marker [268]. In practice, these volatiles are often produced in low concentrations and need a long accumulation period to become detectable. This accumulation period will influence the metabolic processes in the fruits, which in turn will respond with the emission of certain volatiles affecting the neighboring fruits.

When unfavorable storage conditions and/or food processes are detected, it is highly desired to have a monitoring system that can provide automated alerts to enable timely and effective interventions by customers to:

a. reduce fresh food product loss during storage by 50% (absolute reduction of 5% of total food lost in storage);
b. extend the storage lifetime of fresh food products by 20%;
c. reduce the use of chemical treatments of fresh food products by 50% (less need due to optimal storage);
d. reduce storage energy consumption by 10%.

These advantages, if achieved, represent major value propositions for substantially improving the sustainability of the fresh food supply chain. The above target values (a), (c) and (d) are defined by the industry based on scientific research [269–272] and the current practices applied by commercial storage using alternative indirect dynamic controlled atmosphere (CA) technologies (b) [273], respectively.

Current and future challenges

Optimizing storage conditions without using any disruptive or invasive methods for monitoring the hermetically sealed storage facilities is a major challenge. Existing monitoring systems can detect indirect anaerobic fermentation (a late process when dynamic CA is applied), but earlier occurring processes (e.g. damage, rotting and ripening) cannot be detected. This means that adjustments to the storage conditions or sending the products to the markets are often initiated too late.

Therefore, a multi-species sensor, which can continuously monitor the gas species during storage (figure 23), offers a huge advantage for early detection of undesirable conditions and could prevent a large amount of fruit being wasted.

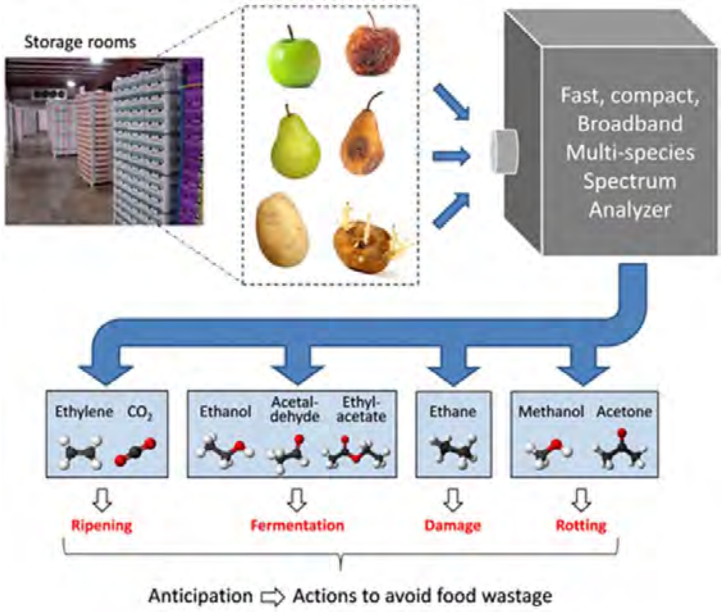

Figure 23. Interactive monitoring of the multi-species volatile indicators released by fruit in controlled storage conditions is the key to preserve the quality of agro-products and prevent losses during prolonged storage.

- Currently, there are three types of technologies available that can monitor these gases.
- Non-optical-based laboratory instruments: gas chromatography and mass spectrometry (e.g. SIFT-MS, PTR-MS).
- Non-optical-based small-size sensors: electronic noses and electrochemical sensors.
- Optical-based sensing systems: nondispersive infrared (NDIR) gas analyzers, fluorescence detectors, FTIR-based instrumentation and laser-based absorption spectroscopy.

The non-optical-based laboratory instruments are complex and too expensive for the real-life application. The NDIR gas analyzers are insensitive and limited to the detection of high concentration levels. Electronic noses, electrochemical sensors and fluorescence detectors can be found in fresh food storage facilities, but these usually have low sensitivity and are not very selective. The laser-based sensing systems using tunable diode laser or quantum cascade (QCL) [274] are a good candidate, although they can only detect one or two species. The detection range can be extended by using more complex sources, such as external cavity QCLs and frequency combs [275].

A mature and inexpensive ultra-broadband light source emitting in the mid-IR wavelength range—where most of the important species demonstrate distinct and strong molecular absorption features—can be the most suitable solution. The mid-IR supercontinuum (SC) light sources are spatially coherent and can deliver higher spectral brightness compare to the alternative thermal sources. These features make them an excellent candidate for monitoring various species simultaneously and with high sensitivity. Using a SC source and a broadband spectrometer (e.g. FT spectrometer—FTS or grating-based spectrometer—GS), one can develop a single analyzer that can cover all targeted species, instead of using a single species sensor for each species. This reduces the overall cost of the sensor system, simplifies the maintenance and unifies the processing control and decision-making. In addition, using such a broadband source, other species can be added to the detection list, thereby increasing the applicability of the system.

Advances in science and technology to meet challenges

We recently demonstrated a mid-IR SC source (NKT Photonics, Denmark) coupled with a grating-based spectrometer (GS) to achieve a spectral coverage of 950 cm^{-1} (2550–3500 cm^{-1}) and a spectral resolution of 2.5 cm^{-1} [276]. The GS is a very popular broadband detection system due to the low cost. Moreover, it is easy to use and provides sufficient spectral resolution for atmospheric gas detection using a single-point detector while scanning the grating. When combined with an absorption multi-pass cell that enhances the effective optical path length and a lock-in detection scheme that increases the signal-to-noise ratio, sub-ppmv sensitivity to various hydrocarbons, alcohols, and aldehydes can be obtained [277].

We developed a multispecies trace gas sensor based on this proof-of-concept and it is currently being tested in small fruit storage facilities. The end product of this multiphase development is an innovative

Figure 24. The journey from a research idea towards a commercial prototype.

interactive storage system that measures the atmosphere of different storage rooms in a storage facility, obtains the concentration of existing volatile markers (i.e. the seven volatile indicators of the health status of the fruit) and translates it into alarm signals/actions for the fruit owner (figure 24). Reaching this level of technology, from a lab setup up to a commercial prototype, required several iteration steps of the functional parts, each with its own specific challenge.

Recent advances in the development of mid-IR SC sources have enables the expansion or their bandwidth from 2 μm to 10.5 μm and beyond [278]. This opens up new possibilities for simultaneous detection of even more gas species with minimum spectral interference, especially when combined with a FTS. Compared to a GS, the FTS is more complex and expensive, but it provides a simultaneous ultra-broad spectral coverage and it is inherently calibrated [279]. However, the newly developed SC sources still need to become more robust and less noisy, which is essential for the SC-based sensor to successfully enter the fruit storage market. Equally important is that the SC source price is reduced by nearly 50% by developing new non-PM pump laser technology. Encouraging progress has been made in this direction and is ongoing.

Concluding remarks

Detection of relevant volatiles for ripening, fermentation, rotting and damage in fruit storage units allows timely and effective interventions when unfavorable conditions occur.

A multi-species gas sensor, based on a mid-IR SC source combined with a GS, has been developed and has demonstrated its ability to monitor automatically and continuously important volatiles emitted by fruits in real-time. The prototype is currently being commercialized. Multidisciplinary technological developments are underway, to further transform the sensor into a commercial interactive storage monitoring and warning system. This will be the world's first automated multi-species gas sensor for fruit storage facilities.

Acknowledgment

The authors thank the Interreg North-West Europe program (Project Number: NWE 363), Horizon 2020 research and innovation programme (Max-Fresh Project No. 958840) and the Netherlands Organization for Scientific Research (Project Number: 14709). The authors would also like to thank Ole Bang from DTU/Norblis and NKT Photonics for the technical support of the mid-IR SC light source.

15. Fluorescence spectroscopy in agri-food chain

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Status

Fluorescence techniques have been used in agriculture and food research for several decades, and have many successful applications [280]. Fluorescence is emission of radiation by molecules, which after excitation by absorption of photons from UV or visible range, return from electronically excited singlet state S_1 to the ground electronic singlet state, S_0. An emission in the visible spectral range may be observed as a glowing color by the naked eye, therefore the early applications utilized visual observation of fluorescence induced by UV light to assess quality of some food products. Due to the high sensitivity and selectivity, fluorescence is particularly useful for studying minor and trace components in complex matrices.

Fluorescent components (fluorophores) naturally occur in plant and animal tissues, contributing to their autofluorescence [281]. This autofluorescence of biological material provides information not only about fluorophores, but also about other relevant properties of sample matrix and has been increasingly used in agri-food sector. Fluorescence techniques are used to monitor the environment, crops and breeding, food processing and to control products safety and quality in the entire agri-food chain.

Fluorescence spectroscopy has been used in monitoring of dissolved organic matter (DOM) in water from natural reservoirs, drinking water and wastewater and detection of water pollution [282, 283]. Fluorescence enables evaluation of water treatment performance, characterization of DOM and monitoring micropollutants and disinfection by-products [284].

Chlorophyll fluorescence emitted by plants has a wide range of applications in monitoring and controlling vegetation processes [285]. It is used as an indicator of PSA and plant self-protection mechanism. Chlorophyll fluorescence is related to the amount of phenolics in the epidermis of leaves and fruit peels, enabling indirect quantification of these compounds [286]. The fluorescence techniques provide information about plant nitrogen (N) status and are applied for the N fertilization management of agricultural crops [285].

Fluorescence sensors have been used for the non-invasive, on-line monitoring of food processing. The changes in the concentration of biogenic fluorophores, observed during microbial cultivation and processing, are applied in biotechnology and food process engineering for process characterization and optimization [287, 288].

Fluorescent food ingredients include aromatic amino acids, polyphenols, fat-soluble vitamins A and E and water-soluble vitamins B_2 and B_6, as well some coenzymes. Many food additives, synthetic dyes and antioxidants, process-derived compounds, some food contaminants and adulterants also show fluorescence [280, 289]. Fluorescent compounds serve as the quality indicators of food, they are related to nutritional value, bioactive functions, sensory attributes, authenticity, processing and shelf life of products [290].

Current and future challenges

Some issues and challenges related to the wider use of fluorescence in the agri-food sector are presented in figure 25. They include development of appropriate measurement techniques, instruments, data analysis methods and applications regarding specific analytes in selected matrices of agricultural and food samples.

One of the important issues is the availability of instruments, which enable acquisition of appropriate fluorescence signals on site, in simple, fast and preferably non-destructive way. The limitations of currently used instruments, hinder usage of fluorescence in on site applications [286].

Several indices based on the fluorescence intensity ratio measured at specific excitation and emission wavelengths have proved to be useful for characterizing fluorophores in plants and food product. Such types of measurements are popular in-field sensing applications, which utilized simple devices. However, measuring fluorescence spectra allows obtaining more amount of relevant analytical information about the examined samples. Biological samples usually contain several fluorescent ingredients, and their autofluorescence provides a characteristic fingerprint. More advanced measurement techniques include excitation-emission matrix (EEM) fluorescence spectroscopy, synchronous fluorescence spectroscopy (SFS), and total SFS [291]. An EEM consists of a set of emission spectra, each of which is measured at a specific excitation wavelength. It presents fluorescence intensity as function of excitation and emission wavelengths and provides comprehensive fluorescence landscapes of the sample under study. The SFS method is based on

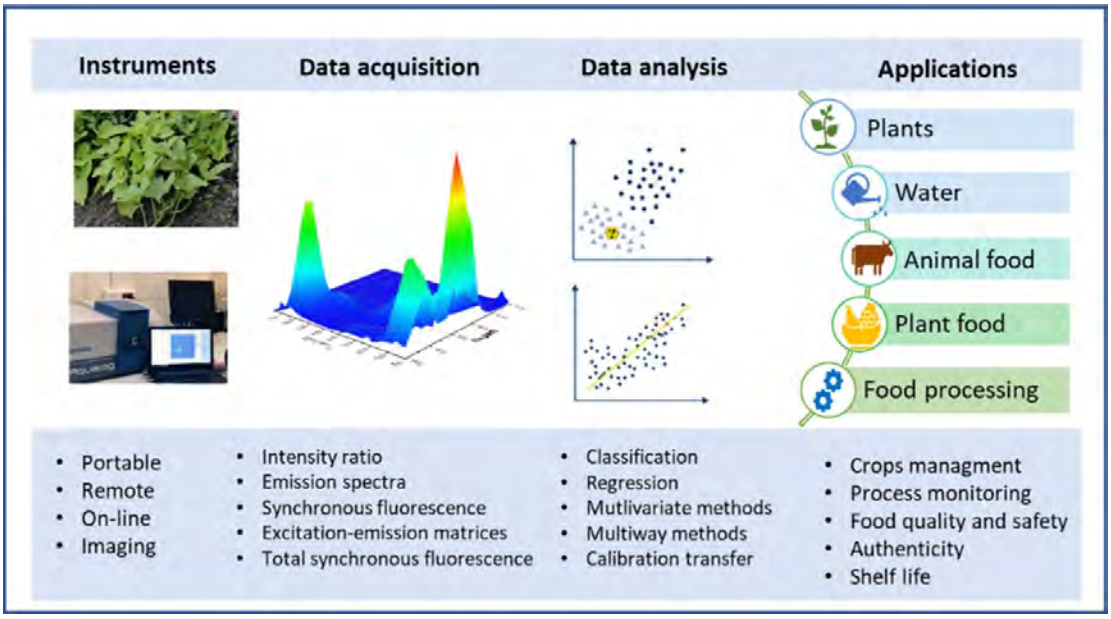

Figure 25. Challenges related to the use of fluorescence techniques in the agri-food sector.

the recording of the spectrum by simultaneous scanning of excitation and emission monochromators, most commonly with a constant wavelength offset, $\Delta\lambda$, between them. TSFS relies on the collection of the set of SFSs. Each SFS is measured at its individual $\Delta\lambda$ value, which varies between scans by a constant value.

To enhance the utility of fluorescence in analysis of heterogeneous samples the imaging techniques are developed, that enable simultaneous obtaining the spectral characteristics and spatial distribution of fluorophores [286]. An alternative to steady state fluorescence measurements may be time resolved techniques. Lifetime measurements eliminate problems with spectral band overlap from different fluorophores and the issues of internal filter effects [292].

The analysis of fluorescence spectra is conducted using advanced multivariate or multiway methods. The unique feature of EEM is the possibility of it decomposition using parallel factor analysis (PARAFAC) [293]. This method provides information on the relative concentrations of each fluorophore present in the sample and enables the determination of their excitation and emission spectral profiles. The results obtained from PARAFAC analysis combined with univariate regression enable direct quantification of analytes in the sample, even in the presence of uncalibrated interferences. This is the so-called 'second-order advantage'.

Advances in science and technology to meet challenges

The development of new instruments and measurement techniques expands the possibilities of using fluorescence in the agri-food sector. Various sensors and imaging instruments are commercially available for measurements of chlorophyll fluorescence and monitoring PSA [286]. The measurement technique include steady-state and time-resolved fluorescence spectroscopy, and pulse-amplitude modulated (PAM) fluorescence. They measure fluorescence excited by controlled light source and are largely limited to the subcellular and leaf levels. This limitation is overcome by development of solar-induced fluorescence techniques, which enable detection of chlorophyll fluorescence excited by sunlight. These techniques enable remote sensing of large area and open new opportunities in agriculture [294].

The important role in miniaturization of fluorescence instruments for on-site applications has played the development of laser-induced fluorescence (LIF) and light emitting diode-induced fluorescence (LED-IF), which replace the conventional light sources [295]. LEDs are compact, available in a broad range of wavelengths and appropriate power outputs, and affordable. The development of analytical applications of miniaturized devices requires the development of methods for calibration transfer between a master bench top instruments and portable fluorimeters based on light-emitting diodes. New solutions in this area can be brought by the use of deep learning methods [296].

The applications of EEM have been extensively increase in the agri-food sector, but fast recording of EEMs remains a challenge [295]. Different solutions have been proposed to solve this problem. Commercially available, filter-based BioView sensor equipped with optical light guides enables rapid acquisition of EEMs for direct monitoring of bioprocesses, however is characterized by relatively low resolution [287]. Recently, a new approach has been proposed to reconstruct of high-resolution EEM from low-resolution data using deep learning super-resolution techniques [297].

For fast, high-resolution EEM measurement, an ultrafast CCD detector can be used instead of a standard photomultiplier. This technology is used in the commercially available Aqualog spectrofluorometer. The instrument is designed for measurements using the A-TEEM technique, which allows simultaneous, fast acquisition of absorbance and transmission spectra, and fluorescence EEM [298].

Hadamard-transform (HT) multiplexing of the excitation light using a programmable light source combined with advanced data processing has recently been applied to reduce the EEM acquisition time [299]. Based on the same HT approach, a four-dimensional fluorescence imaging system was developed, in which each of the pixels in the image array contains an EEM [300].

In parallel with the development of instrumentation techniques, new data analysis methods are developed, which allow obtaining analytical information using the unique multidimensional nature of fluorescent signals [301]. An important element in the development of applications of fluorescence methods is data interpretation. For this purpose, it is important to develop and make available databases presenting fluorescence spectra of various relevant fluorophores and categories of agri-food samples in a systematic and standardized way.

Concluding remarks

Fluorescence, like other spectroscopic techniques, is simple and fast, allows direct and non-destructive measurements and simultaneous determination of many fluorophores. The unique properties of this technique are its high sensitivity, good selectivity and multidimensional nature. The study of plant and animal tissues and raw and processed foods is based on the analysis of their autofluorescence, associated with the presence of fluorescent components. Fluorophores in food include components derived from the raw material, compounds derived from the process, and fluorescent additives, contaminants, and adulterants.

Many studies and some successful applications indicate a great potential for the use of fluorescence in the agri-food sector. However, most of these studies are still in the laboratory phase and there is a large gap between the academic, laboratory scale and industrial applications. Research should focus on better characterization of fluorophores found in different groups of raw and processed food, as well as modeling and understanding the relationship between autofluorescence and the relevant properties of the tested material. The use of fluorescence methods in agriculture, production, processing and food quality control depends on the further development of portable devices and the use of modern ITCs to collect and analyze data from these instruments. Developments in these areas should contribute to the widespread use of fluorescence methods as a valuable analytical tool in managing the agri-food supply chain.

16. Laser-induced fluorescence spectroscopy for mycotoxin detection in solid food products

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Status

The development of rapid, sensitive and non-destructive Mycotoxin sensing techniques is of indispensable importance to enhance food safety and quality. Mycotoxins, being secondary metabolites of toxic fungi, appear on a wide range of food and feed products imposing severe health risks, while they cannot be destroyed or removed by food processing and are invisible for the human eye [302–304]. To safeguard human and animal health, worldwide regulations setting maximum values for mycotoxins in food and feed are in place [305]. These maximum allowed contamination levels show regional variations, as well as vary dependent on the toxicity of the mycotoxin-type and the considered food products. Considering aflatoxins, the European Commission puts a limit of 4–15 μg kg^{-1}, while for ochratoxin and zearalenone the limit ranges between 0.5–10 μg kg^{-1} and 20–400 μg kg^{-1}, respectively [306]. Traditionally, chemical analysis, including liquid chromatography-dual mass spectrometry (LC-MS/MS), are applied to determine the mycotoxin contamination in food and feed products [303, 304]. Despite being highly sensitive and accurate, these chemical analysis might unfortunately give a truncated view on the contamination within a batch by measuring the mean contamination level instead of the local one, while also being destructive and thus inducing food waste.

Fluorescence spectroscopy has been identified as a promising non-destructive alternative for the detection of fluorescent mycotoxins, including aflatoxin, ochratoxin and zearalenone [307–311]. Traditional fluorescence spectroscopy typically considers one-photon induced fluorescence (OPIF) where the fluorescence emission results from the absorption of a single photon. OPIF has shown a promising detection within a wide range of food applications, not only limited to mycotoxin sensing, but also for foreign object detection and food quality evaluation [289, 312]. As main disadvantage, OPIF typically excites different natural fluorescent elements in the food products causing strong background signals. Two-photon induced fluorescence (TPIF), based on the simultaneous absorbance of two photons to excite the electron that subsequently relaxes to emit the fluorescent photon, has been launched as a possible technology to achieve a more selective excitation. Application of TPIF has been demonstrated for the sensing of mycotoxins in alcoholic beverages and maize kernels, as well as for chlorophyll [313–316]. For both OPIF and TPIF, the electron energy transitions are determined by the bandgap given by the Jablónski diagram, dependent on the chemical structure of the product. OPIF typically requires UV excitation wavelengths, while TPIF uses NIR light. TPIF, due to its non-linear character, requires significantly higher excitation powers than OPIF. In addition, according to the quantum physics selection rules, two-photon absorption is not allowed for every molecular structure, implying that not all molecules emitting OPIF generate a TPIF signal when excited with the double wavelength and sufficiently high excitation power density [317, 318]. Non-centrosymmetric molecules enable both one-and two-photon absorption, while for centrosymmetric molecules this transition is allowed for either OPIF or TPIF. In addition, the molecular structure influences the possible electron transitions. Strong two-photon absorbing molecules typically show strong donor and acceptor groups in combination with a long π-conjugation system, since this enhances the nonlinearity in the system and increases the potential for charge-transfer.

Current and future challenges on the application of one-and two-photon induced fluorescence

Application of one-and TPIF for food evaluation requires tackling the following challenges: (1) optimization of the excitation wavelength maximizing the fluorescence of the element under study while minimizing the background fluorescence, (2) optimization of the excitation power density maximizing the signal to noise ratio, (3) extensive validation taking the natural variation into account, both harvest and area dependent, (4) sensitivity optimization to comply to the global legislations, (5) careful product sampling tackling the inhomogeneous presence of the toxin on the products.

Aflatoxin shows both OPIF and TPIF (figure 26), as illustrated for pure aflatoxin B1 powder (purity >98%, A. flavus fungi, Sigma-Aldrich). Pure aflatoxin B1 features a strong absorption around 365 nm, motiving the choice for this excitation wavelength during OPIF, while an excitation wavelength of 730 nm is used during TPIF [314]. Both OPIF and TPIF spectra show a maximal fluorescence intensity at 428 nm

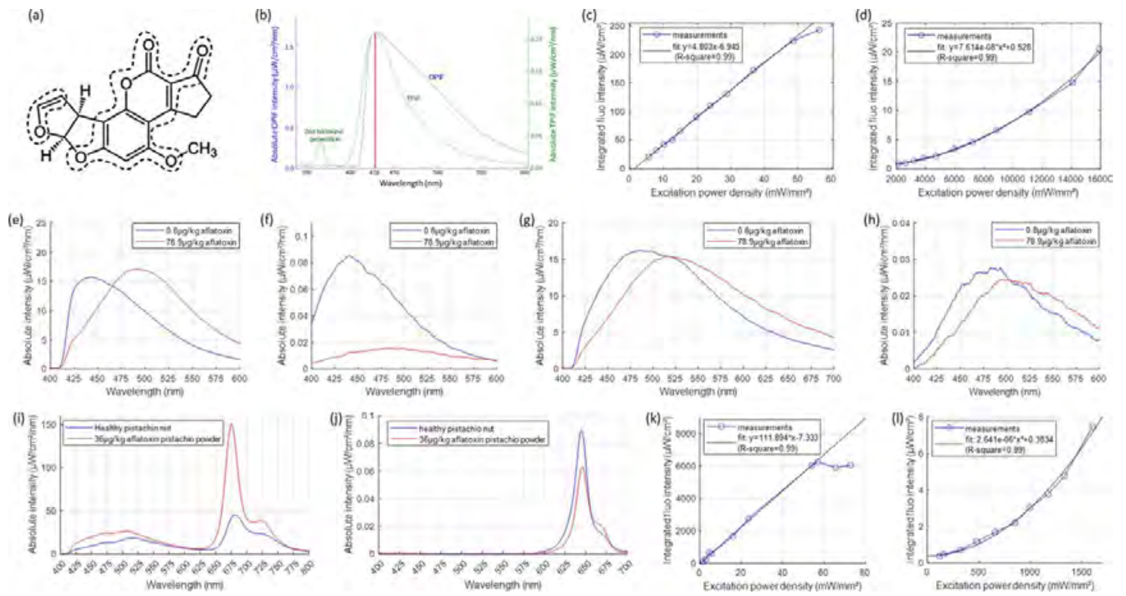

Figure 26. (a) Aflatoxin B1 molecular structure, (b) OPIF and TPIF spectrum of pure aflatoxin B1 powder, (c) aflatoxin OPIF and (d) TPIF as function of excitation power density, (e) OPIF of maize kernels for an excitation wavelength of 365 nm, (f) TPIF of maize kernels for an excitation wavelength of 730 nm, (g) OPIF of maize kernels using 405 nm as excitation wavelength, (h) TPIF of maize kernels using 810 nm as excitation wavelength, (i) OPIF of pistachio with excitation wavelength 385 nm, (j) TPIF of pistachio using an excitation wavelength of 740 nm, (k) OPIF and (l) TPIF of pistachio as function of excitation power density.

(figure 26(b)). The TPIF spectrum shows a narrower peak than the OPIF spectrum, due to the more selective excitation during two-photon absorption. Furthermore, the TPIF spectrum shows a second-harmonic generation (SHG) signal at 365 nm, created by the recombination of two illumination photons to a new photon with the double energy. The aflatoxin fluorescence signal as function of the excitation power density shows a linear behavior for OPIF, until the saturation point is reached where all electrons are excited to the higher energy state (figure 26(c)), while a quadratic dependence is observed for TPIF (figure 26(d)). Aflatoxin contaminated maize kernels indicate a wavelength shift within the fluorescence emission increasing with the contamination level (figures 26(e) and (f)), while showing a stronger contrast for TPIF than for OPIF [315]. Detuning the excitation wavelength from the optimal aflatoxin absorption, using 405 nm and 810 nm for OPIF and TPIF, results in a decreasing wavelength shift (figures 26(g) and (h)).

Considering pistachios, the aflatoxin presence influences the OPIF background fluorescence around 475 nm (figure 26(i)). To maximize the fluorescence signal, and aflatoxin detection with respect to the natural fluorescence, re-optimization of the excitation wavelength was required [319]. TPIF showed to be less suitable for aflatoxin detection in pistachios, illustrating the complexity of the TPIF selection rules (figure 26(j)), while still showing a strong chlorophyll TPIF signal between 600 nm and 675 nm. Studying the fluorescence intensity as function of the excitation power density confirms the linear and quadratic behavior for OPIF and TPIF, respectively, while indicating the higher illumination power constraints for TPIF (figures 26(k) and (l)).

Ochratoxin A shows a similar behavior as aflatoxin (figures 27(a)–(d)), but featuring the strongest fluorescence signal after excitation using 356 nm and 710 nm, for OPIF and TPIF, due to its difference in absorption characteristics. Similar excitation power constraints can be observed as for aflatoxin (figure 27(d)). Zearalenone only shows OPIF, while two-photon absorption only induces SHG (figures 27(e) and (h)). The absence of the TPIF signal can be explained by the study of the molecular structure of zearalenone, showing a much shorter π-conjugation system than aflatoxin B1 and ochratoxin A (indicated by the dotted curves in figures 26(a), 27(a) and (e)), while featuring a smaller amount of donor and acceptor groups. Aflatoxin B1 and ochratoxin A contain nine donor/acceptor groups, while zearalenone only contains seven donor/acceptor groups [320].

Advances in science and technology to meet challenges

Fluorescence spectroscopy is currently benefitting from (1) advances in novel light source developments, (2) advanced optical design, (3) miniaturized sensor technologies and (4) AI/ML data processing algorithms.

(1) Traditionally, fluorescence spectroscopy has been performed using laser light as excitation source, featuring a high cost and complicating the miniaturization of fluorescence measurement units. The

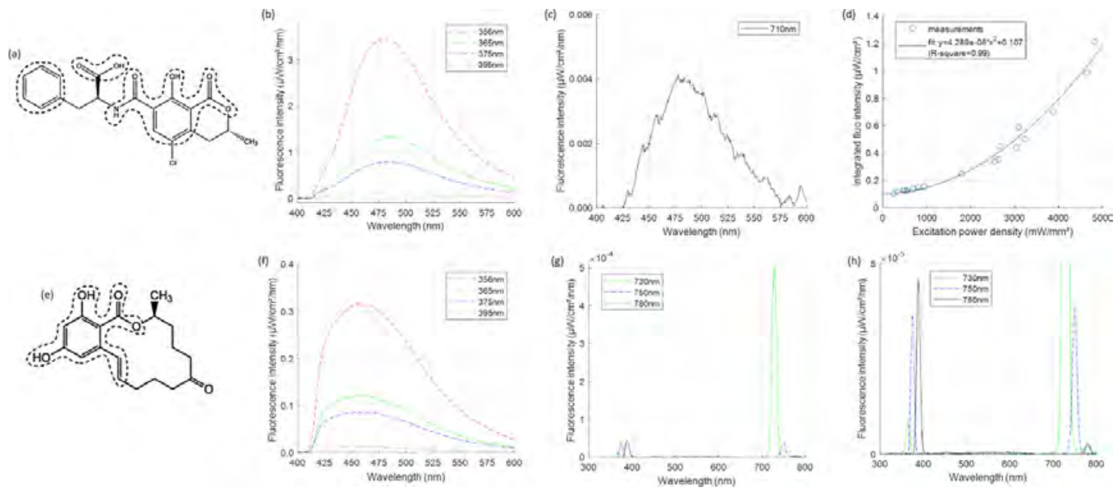

Figure 27. (a) Ochratoxin A, (b) OPIF and (c) TPIF of ochratoxin for different excitation wavelengths, (d) ochratoxin TPIF signal as function of excitation power density using 710 nm as excitation, (e) zearalenone, (f) zearalenone OPIF signal for different excitation wavelengths, (g) SHG of zearalenone during two-photon absorption using different illumination wavelengths, (h) close-up of (g).

ongoing development of high power LEDs, also UV LEDs, drives miniaturization and integration within handheld devices [310]. Although, it should be taken into account that LEDs feature a broader emission spectrum that might induce additional background fluorescence signals, or requires the implementation of additional optical filters.

(2) Advances in illumination and light collection optics, including freeform optical design, benefits the excitation power density, illumination beam properties and light collection efficiencies.
(3) Natural fluorescence emission signals typically show a low emission power, requiring a sensitive detection, which often results in the trade-off between detector size, sensitivity and spectral resolution. The increased availability of miniaturized spectrometer modules benefits the industrial integration of fluorescence spectroscopy.
(4) An ongoing trend towards the use of ML processing and AI models can be observed enhancing the detection algorithms, boosting the sensitivity and selectivity of the instruments.

In addition to the discussed one-and two-photon induced spectral measurement, fluorescence lifetime measurements are being investigated for aflatoxin detection, implying the measurement of time-resolved spectra [321]. However, since this technology requires consecutive fluorescence measurements, it is currently less suitable for in-line and real-time industrial implementation.

Concluding remarks

Fluorescence spectroscopy offers a non-destructive sensing of fluorescent mycotoxins. In general, when considering food products, the mycotoxin fluorescence is not observed directly, but its influence on the natural background fluorescence is monitored. TPIF requires significantly higher excitation power densities and shows lower fluorescence emissions, but might offer a more selective excitation, dependent on the products and the corresponding electron transition selection rules.

17. Raman spectroscopy for precise food quality assessment

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Status

RS is a powerful analytical technique for the quality control of food because it provides specific quantitative information on the chemical composition and on structural information of the substances present, thus representing a molecular fingerprint.

The main advantages of RS are that it is non-invasive, non-disruptive, works also on opaque samples, does not require any sample preparation, has a high specificity, and is fast. For these reasons, RS is emerging as an alternative method to conventional analytical techniques.

RS has demonstrated being able to play an important role in food quality assessment. For example, it was successfully applied to the quality assessment of meat during processing and storing (freezing) [322]. The most useful Raman bands for determining the secondary structure of proteins are those of amide I (1645–1685 cm^{-1}) and amide III (1200–1350 cm^{-1}) while those for lipid monitoring oxidation are at 800–1800 and 2800–3000 cm^{-1} [323]. The analysis of fatty acids is used for the assessment of geographical origin, thermal stability, and adulteration in vegetable oils [324, 325]. The relevant bands correspond to C=C stretching and bending modes, C–C and C=O stretching modes, C–H and CH2 twisting and scissoring modes (in 965–1750 cm^{-1}). In alcoholic beverages and alcohol–water binary systems RS allows monitoring fermentation, detection of counterfeited or adulterated liquors, and discrimination between liquors of similar characteristics [326]. In distilled alcoholic beverages it is essential to monitor the concentration of ethanol and methanol. The ethanol spectrum has one strong band (879 cm^{-1}), assigned to C–C stretching, and two weaker ones (1030, 1079 cm^{-1}) assigned to C–O stretching and CH3 rocking, respectively. Methanol has a very strong band at 1019 cm^{-1}, corresponding to C–O stretching [327]. In fermented alcoholic beverages and yeast fermentation processes the glucose and sugars in addition to ethanol are monitored to optimize the production [328]. This is also true for the analysis of honey since different sugars (fructose, glucose, or cheap sweeteners) are characterized by different bands (in the range 700–1700 cm^{-1}): their relative intensities provide information on adulteration, origin, or physicochemical characterization [329]. In the dairy industry, RS allows to determine intrinsic analytes such as milk components (protein, fats, and lactose) and adulterants and contaminants (non-dairy proteins, microorganisms, antibiotics, and pesticides) [330]. Finally, RS plays an important role in agriculture because it can detect biological and chemical pollutants [331].

Current and future challenges

Despite the large number of advantages, the diffusion of RS in food applications has been hampered so far by two major challenges: the inherently weak signal, which is 10^{-6}–10^{-9} times weaker than Rayleigh scattering, and the presence of fluorescence, which is stronger and broader than the Raman fingerprint and can completely mask it.

To cope with these challenges the conventional approach is to carefully design the optical setup. The most critical decision is the choice of the excitation wavelength. In fact, to reduce or eliminate the contribution of fluorescence, it is advantageous to choose an excitation wavelength in the NIR (typically 785 nm or 1064 nm). This comes to a price, however, since the intensity of the Raman signal is inversely proportional to the fourth power of the wavelength. A further parameter is the laser intensity on the sample since the Raman signal is proportional to the excitation intensity. Unfortunately, food samples are prone to photobleaching and thermal degradation. Therefore, the laser power and the spot size (influenced by the design of the excitation optics) need to be chosen such as to not affect the sample. A further challenge to be taken into account when designing the optical setup is that the correlation between the absolute intensity of the Raman band and the analyte concentration is not always straightforward. The Raman intensity depends not only on the analyte concentration but also on other factors, such as the laser power, optical geometry, and instrumental effects. The most critical of these is the laser stability. To compensate for this effect, strategies include the determination of ratios between intensities of different bands and the use of internal or external reference substances.

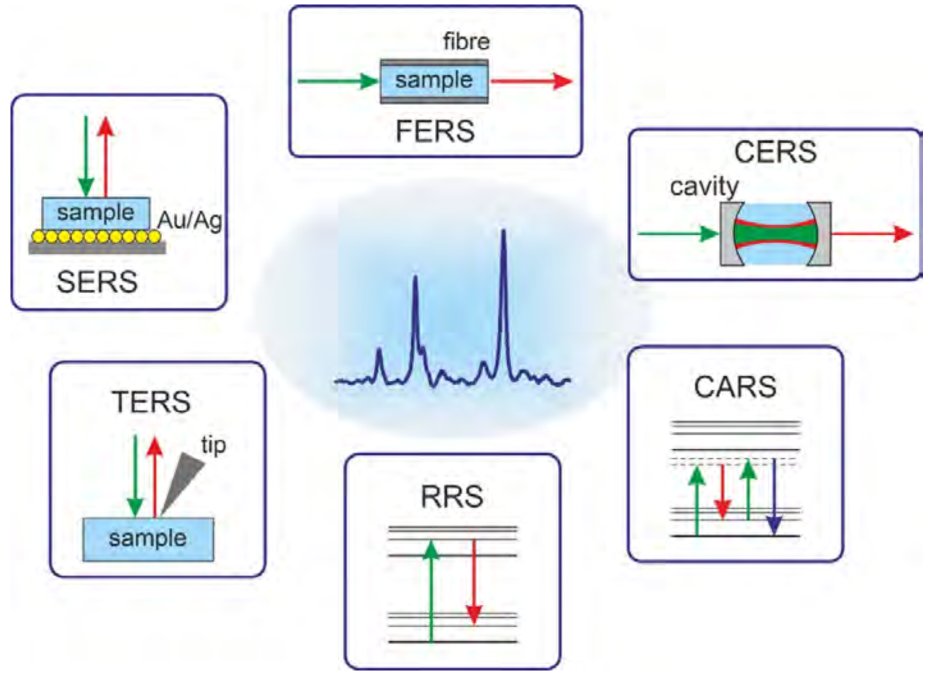

Figure 28. Overview of the most common strategies to enhance the Raman signal. CERS: cavity-enhanced Raman spectroscopy, TERS: tip-enhanced Raman spectroscopy, RRS: resonant Raman spectroscopy, CARS: coherent anti-Stokes Raman spectroscopy, FERS: fiber-enhanced Raman spectroscopy, SERS: Raman spectroscopy.

Finally, an additional challenge is related to the frequent existence of overlapping bands, which influence the spectrum. This makes it difficult to use polynomial-based methods to automatically correct for baseline effects and requires the use of mathematical band-narrowing and resolution-enhancement methods.

These challenges have stimulated a lot of studies on the improvement of the experimental setup including special signal-enhancement schemes and on the development of advanced signal processing techniques, focused on reducing the noise, removing the background (for example due to fluorescence) and extracting the relevant information.

Advances in science and technology to meet challenges

The advances in science and technology can be divided into strategies to improve the signal-to-noise ration by enhancing the weak Raman signal (figure 28) or suppressing the background, and development of post-processing algorithms to extract the desired information from the data.

The most frequent approach to enhance the Raman response is surface-enhanced RS (SERS), which exploits the interaction of the sample with metallic nanoparticles. Similarly, tip-enhanced RS (TERS), a variant of SERS, uses a metallic tip to achieve nanometric spatial resolution. The applications range from the quantification of the relative contents of carotenoids, oleic acid, and phenols [332] to the detection of pollutants, additives, and heavy metals in various food or agricultural products [333, 334].

Other enhancement schemes are based on the choice of special excitation wavelength(s) to achieve resonance effects. These include resonance RS (RRS) and coherent anti-Stokes RS (CARS). RRS, in which the excitation wavelength corresponds to electronic transition, is particularly successful in the analyses of carotenoids and other pigments in foods, whose absorption bands are in the visible. For example, changes in carotenoid concentration can be used as indication of oxidation in olive oil (figure 29) [335]. CARS is a four-wave mixing process, which uses two excitation beams, a pump and a Stokes one, whose energy difference corresponds to a molecular vibrational energy. CARS has been successfully used to distinguish different edible oils and detect their adulteration [336].

In cavity-enhanced RS (CERS) the signal amplification is achieved through the enhancement of the light-sample interaction and laser intensity using multi-pass cells and cavities. Fiber-enhanced RS (FERS) works on a similar basis, with light guided into capillary, fibers and hollow-core photonic crystals. Both techniques, appropriate for gaseous samples, are of great interest to food (postharvest) chain management because they allow to monitor multiple gases simultaneously with one instrument. The most important gases are oxygen, carbon dioxide, and ethylene. These gases play an important role in the inhibition of bacterial growth and the ripening process [337].

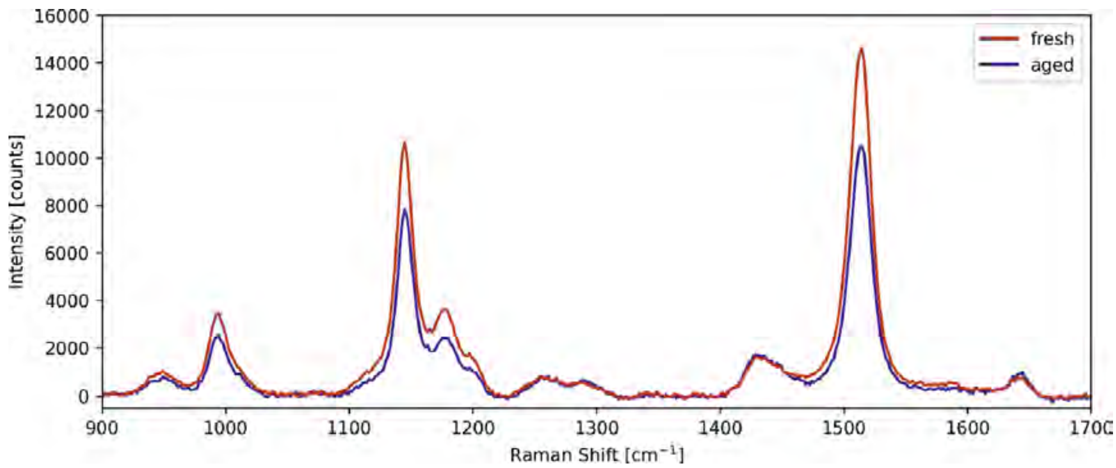

Figure 29. Raman spectra of EVOO fresh and after ageing showing the effect of oxidation on the carotenoids' bands. Reproduced from [335]. CC BY 4.0.

Advancements specifically targeted to improve the signal-to-noise ratio by reducing the fluorescence background include time-gated (TG) RS, which exploits the different time scales of fluorescence and Raman processes, shifted excitation Raman difference spectroscopy (SERDS) and modulated Ramans spectroscopy, which take advantage of the difference in spectral behavior of fluorescence and Raman scattering [338].

The improvements of post-processing algorithms include denoising, and background-suppression algorithms [339]. Due to the complexity arising from overlapping bands, multivariate data analysis methods are frequently necessary [340]. ML is well suited to capture complex relationships within large sets of spectra and is therefore intensively used in combination with most of the previously mentioned enhancement techniques. The newest approaches exploit deep learning for classification and regression tasks [341].

Concluding remarks

Despite the numerous applications already existing, RS still has the potential to become a leading analytical technology for precise food quality control. Its high specificity, non-invasive, and non-disruptive nature provides a quantitative molecular fingerprint which contains information on the chemical and structural information. This is particularly relevant for food analysis, due to the complex composition and variability of substances to be monitored. The advances in the measuring and sampling techniques mentioned before, and the increased availability of components (lasers, detectors) at affordable prices, contribute to the appearance of more and more Raman setups and commercial instruments. This is bringing Raman out of the research lab into the field. The larger datasets available and the advances in algorithm development and deep learning data analysis capabilities additionally push the creation of more sophisticated models. As a result, the adoption of Raman as an analytical tool is expected to achieve a prominent role in food applications.

18. Raman spectroscopy for soil inspection—pathway towards on-site field measurements

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Status

Soil is of global importance in today's agricultural practice to secure the food supply for a steadily increasing population. Detailed compositional information is crucial for protection and sustainable use of soils and can also provide a better understanding of complex soil systems thus generating valuable inputs for on-site decision support tools to control fertilization and irrigation management in PA. Established analytical techniques for soil assessment are mostly based on the collection of mixed specimens from rather large areas (on the order of 10.000 m^2) and have only limited ability to adequately capture the present spatial heterogeneity on agricultural fields. Unfortunately, the expensive, time-consuming and labor-intensive nature of such methods prevents the simple increase of the number of collected samples.

Optical techniques are able to provide a suitable alternative, particularly if they have the capability for field deployment. Element-specific methods, as e.g. X-ray fluorescence or laser-induced breakdown spectroscopy, are valuable tools to determine total mass fractions of a wide range of elements found in soils but they are unfortunately unable to assess the molecular binding form of these elements. Molecule-specific techniques can close this gap by providing information about the soil molecular composition. RS is such a method that is based on the excitation of molecular vibrations within the probed sample thus providing a fingerprint on molecular level. Specific advantages include the capability for rapid, contact-less and non-destructive analysis and low interference by water in the Raman fingerprint range, the latter making the technique particularly suitable for the analysis of soil with varying moisture contents, as e.g. present under field conditions.

The benefits of RS for molecule-specific soil inspection are exploited in a wide range of application areas. Beside the agricultural sector, e.g. for the characterization of phosphorous compounds [342, 343], this also includes soil analysis within archaeological sites [344], investigations of terrestrial analogues in preparation for space exploration [345] and soil forensics [346]. Moreover, Raman spectroscopic studies on soil are reported to assess traffic pollutants in urban soil [347], for the detection of microplastics within soil [348] as well as for the quantification of soil gases [349].

Current and future challenges

Despite the above-mentioned advantages, RS is currently still underexplored in the field of soil science. One major issue is that the weak Raman signals can easily be masked by interference from fluorescence originating from soil organic matter and clay minerals [350]. Selected approaches are proposed to address this fluorescence issue. Mathematical methods for background subtraction are easy to implement but frequently have difficulties in addressing strong fluorescence interference. Microscopic Raman investigations permit to focus on very small areas with diameters around 1 μm and thus enable to diminish the extent of fluorescence from out-of-focus regions. Nevertheless, residual fluorescence contributions can still overwhelm weak Raman signals even when confocal Raman microscopy is applied [343]. Prolonged sample exposure to the excitation laser radiation ('fluorescence bleaching') has the potential to reduce fluorescence intensity but may cause detrimental effects like sample heating, modification or damage. Another possibility to address the fluorescence issue is the usage of deep UV excitation wavelengths below 250 nm that permit for a spectral separation of the Raman signals from the fluorescence emission. However, it is reported that the high energy of the laser photons may cause decomposition of organic matter within the soil, sometimes even when the sample was cooled down to -100 °C [342]. In case of on-site soil investigations, e.g. on agricultural fields, ambient light poses a further challenge to the Raman investigations. This type of interference can also mask the Raman signals of interest and further requires short exposure times to avoid saturation of the charge-coupled device (CCD) detector [351].

For representative assessment of the soil molecular composition, the present spatial heterogeneity at multiple length scales needs to be considered as well. To address the variability on the micrometer scale, a sufficiently large measurement spot size, e.g. 100 μm diameter, is a suitable methods while spatial variations on the millimeter scale can be captured using a raster scan approach, e.g. applying a 10×10-point grid pattern [352].

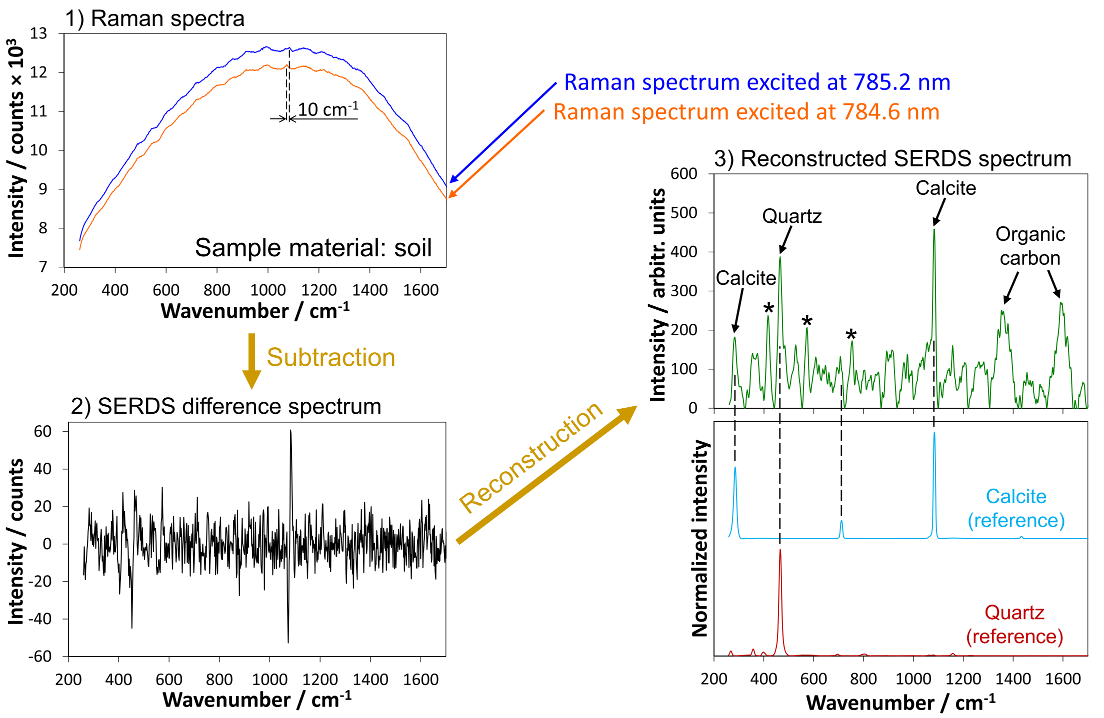

Figure 30. Schematic workflow for shifted excitation Raman difference spectroscopy (SERDS) demonstrated for a soil sample. Two Raman spectra are recorded using two slightly shifted excitation wavelengths (spectral shift: ca. 10 cm^{-1}, corresponding to 0.6 nm at 785 nm excitation). Raman signals follow the shift in excitation wavelength while non-Raman contributions remain unaffected. Subtraction of the two Raman spectra generates a SERDS difference spectrum separating Raman signals from interferences. A SERDS spectrum in conventional form is obtained by reconstruction of the derivative-shaped SERDS difference spectrum, e.g. using numerical integration. Contributions from the soil constituents quartz, calcite and organic carbon can be identified by SERDS, e.g. using reference SERDS spectra of pure materials or literature data. Asterisks indicate Raman signals of the sapphire optical window used to cover the soil sample.

Moreover, the detection of species that are only present at low abundance, e.g. nutrients or pollutants, may be challenging. Here, methods for Raman signal enhancement are beneficial, e.g. SERS, as demonstrated for the quantification of available nitrogen in soil [353] or the detection of pesticides [354]. However, in most cases an extraction procedure is required and the resulting solution (e.g. filtered supernatant) is then brought in contact with SERS-active metal nanoparticles for Raman analysis.

Advances in science and technology to meet challenges

The major challenge of interference by fluorescence and ambient light can effectively be addressed by SERDS [355]. In addition, long excitation wavelengths around 785 nm are particularly advantageous. As shown for selected soils, when using excitation wavelengths above 700 nm fluorescence emission can be much lower compared to excitation wavelengths below 600 nm, thus already enabling a reduction in fluorescence intensity [356]. Moreover, 785 nm is an established excitation wavelength in RS and it still maintains compatibility with sensitive silicon-based CCD detectors. Shorter excitation wavelengths in the red spectral range, e.g. at 671 nm, may be beneficial to access the high wavenumber region with the potential to specifically address organic components or to determine the soil moisture content.

SERDS applies two slightly shifted laser wavelengths, e.g. 784.6 and 785.2 nm, and two Raman spectra are recorded subsequently. Raman signals directly follow the shift in laser excitation wavelength while other contributions remain unaffected. A subtraction of the two Raman spectra thus separates the Raman spectroscopic information from such interferences. To obtain a Raman spectrum in conventional form, the derivative-shaped SERDS difference spectrum can be reconstructed, e.g. using numerical integration. It should be noted that shot noise contributions caused by LIF cannot be removed and are thus carried through into the SERDS spectrum. Nevertheless, soil constituents can be identified based on reference spectra obtained from pure materials as exemplarily shown for the soil minerals quartz and calcite (see figure 30). Originally applied using bulky tuneable laser sources, only the recent availability of compact dual-wavelength diode lasers has unlocked the potential of SERDS for portable instruments [357].

A recent proof-of-concept study highlights the capability of SERDS for detecting the soil constituents quartz, feldspar and hydroxyapatite [358]. Systematic laboratory investigations on 150 soil samples collected from an agricultural field in Germany demonstrate that 13 different soil minerals and amorphous carbon can be detected and that even quantitative analysis is possible, e.g. for the prediction of the soil organic matter [352] or soil carbonate content [350]. The technique is subsequently translated towards the field environment by deploying a portable SERDS system for on-site analysis at selected measurement positions [357].

Based on the successful field study, a modified version of the portable SERDS instrument for the integration into a sensing platform to enable continuous soil monitoring across the field is currently under development. To fully exploit the benefits of the technique, a holistic approach combining sensitive hardware with advanced data analysis methods (ML) and sensor data fusion is pursued. The larger focal depth required for non-contact continuous measurements comes at the expense of increased spot sizes resulting in reduced power density. However, this effect can be compensated by using higher power dual-wavelength diode lasers [359]. During the movement, the two Raman spectra required for SERDS are not recorded at the same position but this issue may be addressed by fast spectral acquisition in the kilohertz range using a charge-shifting technique [360].

Concluding remarks

SERDS is demonstrated as an efficient tool to extract Raman signals of soil constituents from interfering backgrounds, e.g. fluorescence and ambient light. The technique is able to identify and differentiate a wide range of soil minerals (including silicates, titanium dioxides, phosphates and carbonates) as well as organic carbon. Beside this qualitative analysis, the obtained molecular fingerprint also enables quantitative measurements, e.g. as shown for the prediction of the soil organic matter and the soil carbonate content. The development of a portable SERDS system specifically designed for soil inspection opens the avenue for on-site soil assessment directly on agricultural fields. An advanced SERDS instrument as part of a sensing platform for continuous soil monitoring, e.g. across agricultural fields, is currently under construction. The results highlight the capability of SERDS and show great promise to transfer the technique to further applications in the agro-food sector (and beyond). Here, successful proof-of-concept experiments are conducted for the analysis of plant leaves and apples [351] as well as animal feed pellets [361].

Acknowledgment

The authors gratefully acknowledge Maria Krichler for software development, and Lucas Wittenbecher and Thomas Filler for development engineering support. We also would like to thank all involved colleagues from the project consortium I4S (Intelligence for Soil) for sample collection and preparation, and the landowner Golo Philipp for access to the agricultural field. This study is funded by the Federal Ministry of Education and Research (BMBF) within the projects RaMBo (Grant Nos. 031A564C, 031B0513C and 031B1069C) within I4S as part of the funding measure BonaRes (Soil as a Sustainable Resource for the Bioeconomy) and Research Fab Microelectronics Germany—FMD (Grant No. 16FMD02).

19. On-site detection of water pollutants: the potential and limitations of optical spectroscopy

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Status

Environmental pollution is at the heart of most research related to climate change and the European Union focused numerous activities on such a crucial field impacting global health, diversity, and food resources [362]. Detecting water pollutant with optical tools is not an obvious choice since water absorbs most of NIR and mid-infrared (MIR) light, where the main spectral features of organic materials are located. However, photonic methods are known to be versatile providing different and complementary ways to these drawbacks with the advantage of being non-invasive, i.e. the sample is not destroyed, and therefore several optical measurements using similar or different methods can be done consecutively.

Spectroscopic analysis is the study of the response in wavelength of an object to an illumination. The source must therefore be broad (or tuneable), e.g. white light, and a dispersive element, e.g. a grating or a prism, must be used. A reference is also mandatory to normalize the spectra correctly, in the case of water, it can be, for instance, deionized water. The spectral response varies from one pollutant to another, but it is to be noted that most of them present absorption peaks in the MIR range [363].

Nowadays, two main robust methods are driving the research on pollutants having the form of particle or affecting objects that can be further analyzed: RS (which can be extended to surface enhance RS) and FT infrared (FTIR) [364, 365] spectroscopy. Both methods give unique signature of constituents of matter in a reliable way. However, both are laboratory techniques requiring expertise in the measurement operation itself and in the sample preparation, which can be laborious and cost ineffective. Commercial portable and even handheld FTIR and Raman spectrometers have been developed for chemical species analysis of solid-, liquid- and gaseous samples. These have been used for product quality control, e.g. in agriculture, petroleum, pharmaceuticals etc. Unfortunately, FTIR detection of contaminants in water is ineffective because the IR probe radiation is strongly absorbed by water itself. The drawback with RS is the fluorescence of some organic materials in water may dominate the Raman signal, especially when short wavelengths are used as probe. Using longer probe wavelength (SWIR) does not improve the method, because the signal is absorbed within a small layer of water or organic material before reaching a microplastic. Hence, the Raman signal can be weak and problematic to analyze regarding quality of a complex water sample.

Other techniques, like digital holography or fluorescence spectroscopy, can greatly improve the situation in some cases, e.g. the detection of microplastics. Some devices exist for on-field measurements, typically optrodes [366]. They are complex optical devices usually based on chemical transducers allowing, optically, to measure one specific constituent. It means that the amount of optrodes must be multiplied by the number of pollutants to be measured.

Spectroscopic methods are interesting only if one can analyze and understand the detected signals. Methods based on different order of derivatives of measured spectrum, PCA, generalized two-dimensional correlation spectroscopy and nowadays ML, data mining and AI help to obtain faster and more reliable or targeted results [367, 368]. Combining mathematical, physical, and chemical understanding of a sample yields a possible simplification of the measurement methods, which constitutes a great step forward for in-situ measurements.

Current and future challenges

Open water is, by definition, a complex medium in which are present useful nutrients, but also numerous particles of different sizes, shapes, and compositions leading to difficult-to-interpret signals independently on the method used for analysis. Moreover, water can be colored, hazy in liquid form but we also must consider vaporous and solid form of water. In the first one, very thin and light particles can be carried over long distances while in the later form, bacteria and other pollutants can be imprisoned for extremely long periods. Current climate changes make even less stable the equilibrium between what is discarded by humankind in nature, i.e. pollutants, life (fauna and flora) in water bodies, and what is released by melting ice, without counting on the temperature variations affecting the ecosystem, the water flow around the Earth, and the exchange of water between ground and ocean [369]. In other words, more pollutants in water are moving faster.

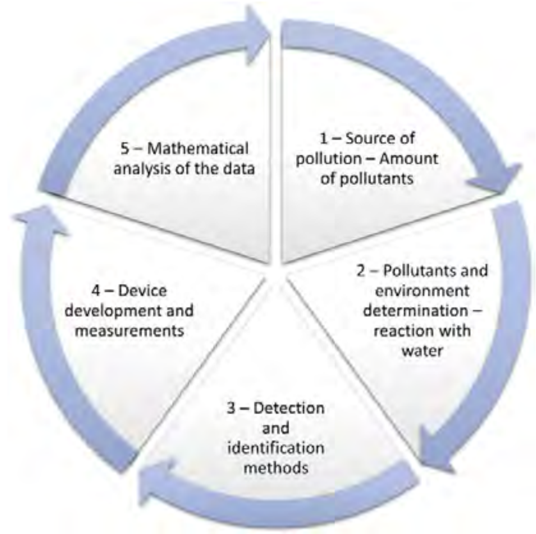

Figure 31. Illustration of a possible scheme to study and understand pollutants in water.

The first challenge one faces in building a device for the detection and identification of pollutants is simply the type of pollutant (figure 31). It can be chemical and completely dissolved in water, which is what happens for instance in case of accidental pollution. An example of future impacting case could be a leakage happening at an energy station supplying the new carburants such as methane and nitrous oxide that can dissolve in water. But pollutants can be particles of a few nanometers or several millimeters such as (micro)plastics, metal, other organics. Pollutants are also, in some cases, complex entities due to a long stay in water, i.e. a particle on which a biofilm has grown and includes bacteria, viruses, other particles. Each of these pollutants requires a specific monitoring technique.

From the optics point of view, it can be a spectral measurement, a transmittance measurement, an imaging of the scattering, or some more complex measurements such as Raman or FTIR spectroscopies. Such methods operate well in limited cases. Typically, when the volume to be analyzed is not too large and the matrix not too complex. It means that some sample preparation (filtering, cleaning, sorting) is required, which makes the work laborious and often expensive. It makes then obvious that another challenge is the volume measurement. Some methods for microplastic detection, for instance, have used dyeing to recognize the particles [370]. Another issue is the portability of the device. It requires light sources, detectors, and robust components which are usually not compatible with accurate spectroscopic measurements.

Finally, VNIR spectroscopy are not always adapted to the analysis of pollutants simply because of the frequency range in which the elements show their main spectral features. However, techniques based on combining both imaging and spectroscopy allows for identification and quantification. Moreover, a mathematical analysis of signals can be done to observe variations corresponding to a specific condition of the monitored environment or an element in it. Usually, such a method is then not sufficient to give a clear identification but allows for very fast screening of large volumes.

Advances in science and technology to meet challenges

New technologies offer advantages that can overcome the limitations of the current devices. We will here name three of them: (1) HSI [371] allows the measurement of a spectrum for each pixel of an image, which means that a relatively large area can be screened at once. It leads to the identification of particles or elements mixed in a liquid, for instance. The price is a huge computational memory and a lack of resolution. This technique has been recently demonstrated has very efficient for the identification of microplastics directly in water [372]. (2) Ultra high-resolution imaging allows counting and localization of particles. Moreover, the method leads to a knowledge of the shape and motion of the particles together with their environment. Unfortunately, the technique does not work for chemicals dissolved in water and does not give a reliable identification of the particles since it often operates at only one single wavelength [373]. (3) LiDARs can probe very large volumes at the price of a lower resolution and a lack of selectivity because of the wavelength [175].

One can see that those three methods are together solving most of the current challenges, and therefore they must be combined. To achieve this, one must have an *a priori* knowledge of the studied environment (reference) and define the problematic to target specific pollutants (database). In this case, one can operate on a few wavelengths which is simplifying the use of LiDARs, allows ultra-high imaging devices, and reduce the memory required by HSI since it will be no longer needed to record an entire spectral cube [372]. For instance, Garaba *et al* state that '1070 nm is the best wavelength to discriminate plastics from extremely turbid water and also determining submerged plastics less than 5 cm' [374].

However, research is progressing rapidly, and combination of techniques and methods is now possible by the novel method of prototyping using 3D printing allowing fast development of light devices, by integrated optics leading to lower needs in power consumption (even power by solar cells) and smaller devices that can be parallelized for more efficient measurements. One short term solution for water pollution monitoring is, for instance, the development of a modular sensor, i.e. a combination of different systems in a modular way, allowing the simultaneous measurement of different pollutants as proposed in the EU project IBAIA [375].

Concluding remarks

Water pollution is due to actions of mankind but also nature, such as, acid rain resulting from eruption of a volcano. Pollution particles in atmosphere can settle down over natural water bodies and oceans. Polluted soil in turn can induce pollution of groundwater sources. This a vicious circle accelerated by the climate change. A difficult and long road towards efficient portable device for spectroscopic measurements remains in front of us. We can however dream of miniaturized compact tools operating at lower power can further be embarked in submarines, boats, buoys, or even on UAVs, or drones, that give access to large area. Systems could be powered by solar or wind energy with data transferred to bigger units for further analysis. The key-solution will certainly come from a multidisciplinary collaboration between researchers in integrated solutions and AI and ML algorithms for a fast and optimized data processing. Often, a compromise must be made to achieve a portable device for in-situ measurements, and this is made through discussions with companies, organizations, and governments taking care of water quality to answer the question of what is the real need? This brings us to the starting point, i.e. the definition of the problematic and the cause of the pollution.

Acknowledgments

This article is based on knowledge acquired over the years working on large consortia projects CEIWA funded by Business Finland (Grant No. 541/31/2021), IBAIA funded by the European Union's Horizon Europe research and innovation programme (Grant Agreement No. 101092723), and the Academy of Finland PREIN flagship (Grant No. 20166).

20. FTIR-based quality control of commodities

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Status

FTIR spectroscopy has a long-standing history in commodity quality control since its first use in the late 1970s [376]. Thereafter, advances in optical components and computing have accelerated the evolution into easier-to-use and affordable FTIR devices establishing the method in a wide variety of application scenarios [377]. Current interest in FTIR spectroscopy in agriculture and food industries is driven by its inherent advantages over conventional dispersive IR technologies, offering improved signal-to-noise ratio, faster data acquisition, multianalyte analysis, and higher spectral resolution [378]. In addition, miniaturization potential of FTIR devices and modern chemometrics/algorithms enables rapid on-site/in-field monitoring of quality, safety, and fraud parameters from wide range of commodities and is nowadays considered a viable alternative vs. conventional chemical methods [376, 379]. While FTIR spectroscopy usually accesses limits of detection (LODs) down to the ppm and occasionally ppb level, several analytical methods based on, e.g. LC-MS are significantly more sensitive. However, these methods are time-sensitive, off-site and require an appropriate laboratory infrastructure and trained personnel [380, 381].

Figure 32 schematically shows the light path within the most commonly used sampling approach in combination with FTIR—attenuated total reflection (ATR) including the radiation source, the ATR assembly and the detector. Using ATR is the most versatile sampling approach in commodity analysis suitable for a wide range of sample aggregate states including liquids, gels, pastes, powders, and homogenized solids.

FTIR spectroscopy is a fast, selective, and non-destructive approach providing access to a 'molecular fingerprint' of the sample facilitating quality control of commodities. This has led to studies applying FTIR technology to a wide range of commodities (e.g. cereals, vegetables, dairy products, fats, oils, nuts, etc.) [378]. Particular interest has focused on using portable and even hand-held FTIR-ATR systems using versatile waveguide-assisted sampling interfaces [379, 383].

The combination of FTIR spectroscopy and chemometrics has been proven as a viable tool for commodity quality control along the supply chain. Spectral databases for specific parameters of commodities can be established harnessing minute variations in the dataset to detect minor alterations [384]. Furthermore, the evaluation process can be automated, thus facilitating high-throughput screening in agricultural applications, and in particular for various commodities. Combining chemometric strategies and FTIR techniques have demonstrated their potential for, e.g. the analysis of proteins in milk and dairy products [385]. Similarly, commodities such as peanuts and maize were investigated within such a screening scenario. A decision tree method proposed by Kos *et al* demonstrated the classification of maize samples at 1750 and 500 μg kg^{-1} thresholds for the mycotoxin deoxynivalenol (DON) resulting from fungal contamination with an accuracy of 79 and 85%, and peanut samples for the mycotoxin aflatoxin B1 (AFB1) at 8 μg kg^{-1} with an accuracy of 77%. This confirms the suitability of the method for classifying samples at the respective regulatory limits [386]. An overview of the reported studies using FTIR for monitoring quality, safety, adulteration, and other parameters in food commodities is given in table 1.

Current and future challenges

The translation of technology from the research laboratory into industry is a crucial step for advancing FTIR technology to be adopted by regulatory measures imposed by respective agencies. From a device perspective regarding portability and design, the transition of FTIR devices from the laboratory into the field addressing real-world samples remains challenging for accurate and reliable commodity analytics. Portable device technology requires miniaturization of optics, overall device dimensions, and the use of correspondingly integrated microelectronics. In addition, bright wideband yet miniaturized light sources and detectors are crucial. Miniaturized interferometers may take advantage of Fabry–Pérot configurations in lieu of conventional Michelson interferometers, yet, always at the trade-off of reduced spectral resolution. Recent advances in light sources (e.g. MEMS-based emitters) and detectors (e.g. pyroelectrics) offer reduced production and overall device costs, albeit at the compromise of increased noise and lower spectral

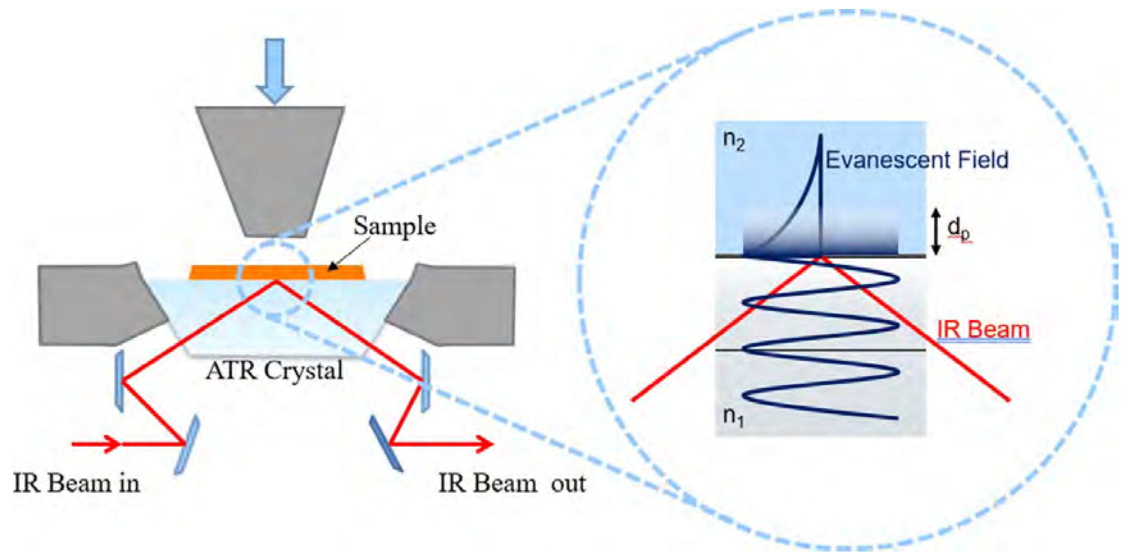

Figure 32. Schematic of a compact Fourier transform infrared attenuated total reflectance (FTIR-ATR) device [382].

Table 1. Selected applications using Fourier transform infrared spectroscopy for monitoring quality, safety, adulteration and other parameters in food commodities. Adapted from Cebi *et al* [383].

Commodity	Parameters analyzed	Equipment	Type of analysis
Cereals	Mycotoxins, proteins, lipids, starch	FTIR-ATR, FTIR	Quality and safety control, authentication
Nuts	Lipids, proteins	FTIR	Quality control, adulteration
Milk	Fatty acids	FTIR-ATR	Safety control, adulteration
Vegetables	pH, °Brix, carbohydrates profile, nitrate, phenols, citric acid	FTIR-ATR	Quality, safety and maturity control, classification
Fats and oils	Total fat, fatty acid composition, fatty acid profiles	FTIR-ATR, FTIR	Quality, safety and adulteration control

resolution. However, if these limitations are addressed more efficient, compact, and versatile portable FTIR spectrometers are certainly feasible [383].

Besides the technology, the application of FTIR devices in agricultural scenarios has its own challenges. The complexity of food matrices limits the discrimination and identification of spectral fingerprints associated with target compounds. This complexity frequently requires complementary sample preparation schemes including but not limited to extraction, purification, and clean-up to separate target analytes prior to the analysis. In addition, spectral information may be extracted using deconvolution techniques and chemometric algorithms [387]. Last but not least, while preconcentration schemes may indeed enhance the sensitivity and reduce interferences and sample matrix effects, several food contaminants need to be detected at ppm-to-ppt concentration levels (e.g. mycotoxins in cereals) requiring outstanding performance of these strategies [388].

Environmental effects (e.g. temperature, humidity, etc.) can negatively influence the spectral data quality, thus data pretreatment strategies are crucial to mitigate those effects and establish sufficiently robust calibration and classification models. A main issue when establishing such models for food analysis are limited and unbalanced datasets and the inherent variability of natural food products. Several studies reported rather sparse datasets to train the associated models, which are of insufficient quality for in-field analysis scenarios [389]. In addition, only few studies include validation procedures to test the robustness of the established models via external samples [390]. Yet, robust chemometric algorithms modeling the variability of commodities and associated matrices can respond to the analytical problems found in food analysis, such as changes in the refractive index at high analyte concentrations, matrix effects interferences and overlapped peaks, natural sample variability, non-linearity between the spectral data and sample concentration and variable selection. Evidently, advanced data evaluation models are crucial to increase the adoption of FTIR-based analysis technologies specifically for commodity analysis, and more generally in agricultural applications.

Advances in science and technology to meet challenges

With a growing world population and shrinking cultivation areas due to climate change and urbanization, safe food supplies remain a grand challenge also in view of increasingly strict regulations and limited resources for food production.

An area reporting significant progress in assistance of analytical techniques such as FTIR-based technologies is ML, which includes the application of robust and innovative data analysis strategies for improved predictions and decisions based on FTIR-derived data. For example, Tsakanikas *et al* [391] developed a high-performance ML workflow for raw food categorization. The workflow was based on PLSs regression and SVM classification for multi-class categorization of seven raw food types. The classification performances obtained exceeded 84% accuracy for the different commodities. Conversely, Öner *et al* [388] tested different ML approaches including adaptive boosting (AdaBoost), Random Forests, SVM, and multilayer perceptron (MLP) for classifying DON-contaminated maize samples at EU regulatory limits with MLP demonstrating $>$91% correctness of the classification. These results confirm that ML approaches are indeed valuable assets for extracting crucial information from FTIR-based data. It should be noted that such algorithms may be implemented on microcontrollers, which facilitates an additional level of device integration in a cost-effective way.

An essential advancement is the development of faster integration times facilitating real-time operations. Real-time analysis is particularly crucial in food processing industries interested in on-the-fly quality control enabling rapid decision-making, production optimization, cost-effectiveness and minimization of waste. With faster integration times and improved chemometric tools, quality parameters may be obtained within a fraction of the time conventional techniques currently require [392, 393].

A major evolution of FTIR technology is the development of portable and even handheld devices. These devices offer on-site capabilities and are ideally capable of considering chemical and biological parameters in complex matrices. Advances in this field should be focused on the development of dedicated analyzers including tailored miniaturized light sources and detectors for specific targets analytes considering constraints related to the required wavelength regime [383, 394].

Another recent development in the field of solid heterogeneous sample analysis is FTIR-based HSI (FTIR-HSI). This technique is particularly applicable to samples such as food powders during industrial processing. By combining the power of FTIR spectroscopy with imaging capabilities, FTIR-HSI enables the analysis of the composition and quality of food products in real-time [395].

Lastly, FTIR micro-spectroscopy has emerged as a valuable tool for analyzing samples at a microscopic level. This technique provides detailed information on the molecular composition of small samples and thin layers with dimensions reaching 10 μm enabling to study commodities at a micro-level [396]. FTIR microscopy allows the identification of inorganic and organic compounds within a sample matrix (e.g. particulates) or the analysis of small commodity particles (e.g. single kernels), which translates into minimum sample requirements [397].

Concluding remarks

FTIR is a well-established spectroscopic technology, yet for the analysis of commodities and monitoring/quality control still an emerging tool. Food industries, agriculture and authorities increasingly demand robust and reliable devices for monitoring food quality parameters in the field, which renders advances in FTIR technology crucial toward adoption as a validated analytical method, e.g. in quality control. FTIR-based techniques advantageously provide rapid data acquisition times, high sample throughput, are reproducible and require minimal-to-no sample preparation. Hence, they are increasingly adopted as a routine tool for but not limited to analyzing food adulteration, food quality, food authenticity and food safety.

The transition of FTIR-based technologies into the food industry hinges on robust spectral data pretreatment, evaluation, and mining, which aid in minimizing sample preparation and separation strategies. ML algorithms have the potential to overcome current data mining limitations toward enhanced accuracy and efficiency, if appropriate trainings data is available. The combination of faster signal integration times with improved chemometric tools potentially allows for real-time operation and on-the-fly analysis.

Packaging advanced data mining technology with portable FTIR systems renders on-site analysis more accessible and user-friendly and allows for operation with non-trained staff. Finally, FTIR HSI facilitates real-time analysis of heterogeneous solid samples. While FTIR micro-spectroscopy provides the molecular composition of minimal sample volumes, particulate samples or single kernels at the micrometer level.

In summary, while being well established in routine analytical laboratories, FTIR spectroscopy may also evolve into a widely adopted molecular analysis technique for controlling and monitoring the quality and safety of a wide range of food and feed commodities.

Acknowledgment

This work was supported by the Europe Union's Horizon 2020 Research and Innovation Programme project PHOTONFOOD (Grant Agreement No. 101016444) and is part of the Photonics Public Private Partnership. This work was partially supported by the Norwegian Research Council through the project SFI Digital Food Quality (Project No. 309259).

21. Optical fiber sensors for precision agriculture

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Status

Due to the continuously growing global population, the demand for food production is constantly increasing, while challenges in the availability and cost of fertile soil, irrigation water and farming nutrients impose additional hurdles. Furthermore, the climate change and the requirement for environmental sustainability constitute the adoption of new and improved agricultural practices a necessity. In this content, the scope of PA is the optimum use of technological innovations in order to maximize agricultural yield while minimizing resources spent [398]. Traditional agriculture is a highly empirical process, whereas PA focuses into the parameterization and optimization of the agricultural practices using new technologies such as sensors, ML and biochemistry. In general, agriculture has been a sector slow in adopting technological advances, with, mainly, traditional agricultural scientists, i.e. agronomists, conveying new tools and methods in the field. However, the aforementioned challenges impose the involvement of specialist from diverse domains such as photonics and information science.

In recent years, various agricultural tasks have substantially advanced by the implementation of PA including field mapping, soil analysis, weather monitoring, labor and equipment management [399]. The wide spread of smartphones and mobile apps, the rapid commercialization of UAVs, the miniaturization of sensing probes and systems, and the suppressed cost of the above due to commoditization, render specific PA technologies a plausible solution even for small scale farms and non-experienced users.

Sensors constitute important parts of the PA value chain, facilitating the direct interaction with the measurands under consideration, while being interrogated in continuous or periodic mode. Optical fiber sensors (OFSs) in particular, is a mature technology with many applications in diverse application fields such as structural health monitoring, biomedical and environmental sensing [400]. OFSs operate remotely, without requiring electrical power at the measurement location, are immune to electromagnetic interference, they have small size and weight, are flexible at installation and induce minimum disturbance. They can provide real time monitoring of parameters and can cover a large area either through distributed measurements, or by exploiting their multiplexing capabilities. Although OFS penetration in PA is still at an early stage, there is great potential and investments in sensors for PA is expected to grow in the coming years.

Current and future challenges

In the last decade, an increasing number of reports have been published on the development of OFSs for PA, encompassing a broad range of agricultural practices such as soil and irrigation assessment, plant growth monitoring, pathogen tracing and measurement of elemental nutrients, while exploiting a number of different optical and transduction schemes.

The irrigation process is instrumental for crop production, simultaneously impacting water resources sustainability, thus soil moisture constitutes a key parameter in PA. Different OFS techniques [401] have been examined, for soil assessment, including an optical fiber distributed temperature sensor that determines soil moisture through the thermal response of a buried optical fiber cable which is subjected to heat pulses [402]. Leone *et al* [403] have reported on a temperature compensated fiber Bragg grating humidity sensor, measuring soil volumetric water content values between 0% and ∼37% employing a polymer micro-porous membrane and a functional packaging (see figure 33(a)). In the area of plant pathogen monitoring, an optical fiber distributed acoustic sensor aided by convolutional neural network (CNN) models was developed for the early detection of red palm weevil in large farms [404] (see figure 33(b)), while detection of Tomato leaf curl New Delhi virus (ToLCNDV) DNA has been presented using a localized surface plasmon resonance based U-bent fiber optic sensor [405]. Following the endorsement of drones in chemical pesticides field spraying, a long period grating OFS has been proposed for tracing spraying droplet distribution [406].

Optical fibers have also been proposed for observing plant growth and evaluating nutrient strategy results since, compared to destructive sampling, they offer a quick and less costly alternative. Indicatively, reports exist on the use of OFS to determine calcium concentration within hydroponic nutrient solutions [409] and macro-nutrients such as total nitrogen (TN) in soil [410]. Promising examples of OFSs have also been demonstrated to actively measure plant growth. This approach applies to both underground measurements, for imaging of plant root growth using a distributed strain fiber optic sensor [411], and

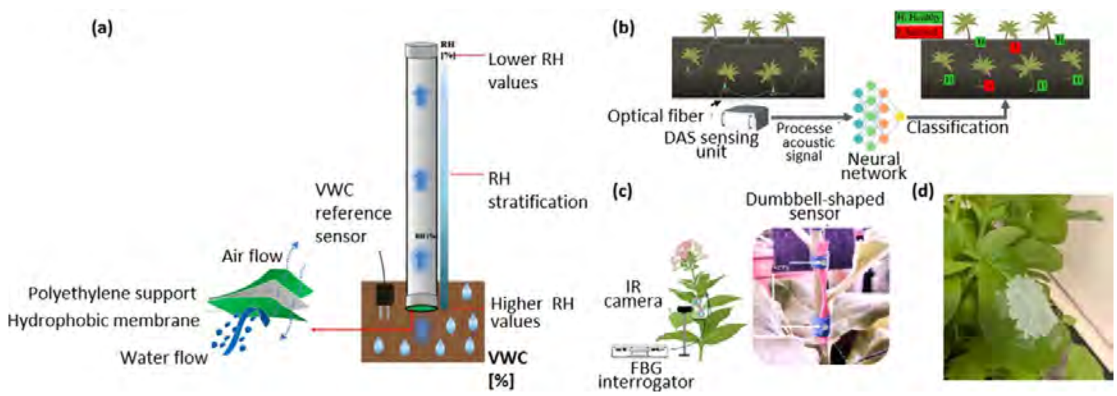

Figure 33. (a) Sensing principle of fiber optic thermo-hygrometer for soil moisture monitoring. Reproduced from [403]. CC BY 4.0. (b) Approach for Red Palm Weevil detection using optical fiber distributed acoustic sensing and machine learning. Reproduced from [404]. CC BY 4.0. (c), (d) Different configurations of wearable Bragg gratings sensors for plant growth monitoring. Reproduced from [407]. CC BY 4.0. © [2023] IEEE. Reprinted, with permission, from [408].

on-specimen wearable sensors based on fiber Bragg gratings in different configurations [407, 408] (see figures 33(c) and (d)). Furthermore, OFSs well established in other major application fields e.g. structural health monitoring are also adopted within PA practices. For example, OFSs designed for structural health monitoring are employed for detecting leakages in water pipes of irrigation systems [412], or damages in agricultural structures [413].

Advances in science and technology to meet challenges

The penetration of OFSs in the now-emerging and multi-disciplinary field of PA is dependent upon three major conditions: functionality, operational characteristics and cost of the developed sensors. Functionality will define the applicability of OFS designs into specific agricultural practices, while exploiting existing or new transduction mechanisms. It is expected that OFSs will be able to provide multi-parametric information -not being available before- in processes such as pesticide spraying, insect monitoring, thermal stress and nutrients circulation, readily providing unique insights to the farmer/agronomist that otherwise would require years of observation (see figure 34). Low cost, reliable probes with simple operation and interrogated by smartphone/tablet based read-out units are cornerstone characteristics that will enable agronomists and non-specialized farmers to utilize OFSs, maximizing their impact to the agricultural community and relevant market sectors. Such a broader adoption of OFSs into PA will allow farmers and agronomists to trace crucial parameters of their crops and fields, accelerating good practices related to prevention of harvest losses, optimal and sustainable use of resources and increase of production rate/profit.

The successful evolution of OFSs into PA is expected to lead to the realization of sensors that will monitor in-situ important functions (i.e. solar radiation, growth, hydration, or photosynthesis) at the crop, plant or tree, inaugurating the protocol 'fiber-to-the-tree (FttT)'. Future FttT OFSs may be realized in the form of needle or attachable pad, possibly exhibiting biodegradable functions [414], and will provide indispensable information on the impact of common agricultural practices, in conjunction with data collected from other OFSs, placed in air or into the soil around the specimens. OFSs, spatially dispersed over a large field, may operate over a fiber-wired or wireless grid, setting up an IoT sensing network for PA (figure 34). FttT OFSs may fuse technologies from Optofluidics [415], Optoacoustics, ML, and new Bio-/Chemo-sensing transduction materials, operating from the visible up to the far-infrared bands [416], where complex spectral signatures can be used for tracing substances with higher specificity. Well studied optical platforms such those of Bragg and long period gratings, plasmonics, microstructured, multi-core and polymer optical fibers, and resonators (i.e. Fabry-Perot, ring, etc) can be used for developing OFSs that will offer measuring capabilities in the open field which have been available only in laboratory environment before [417], thus revolutionizing the field of PA.

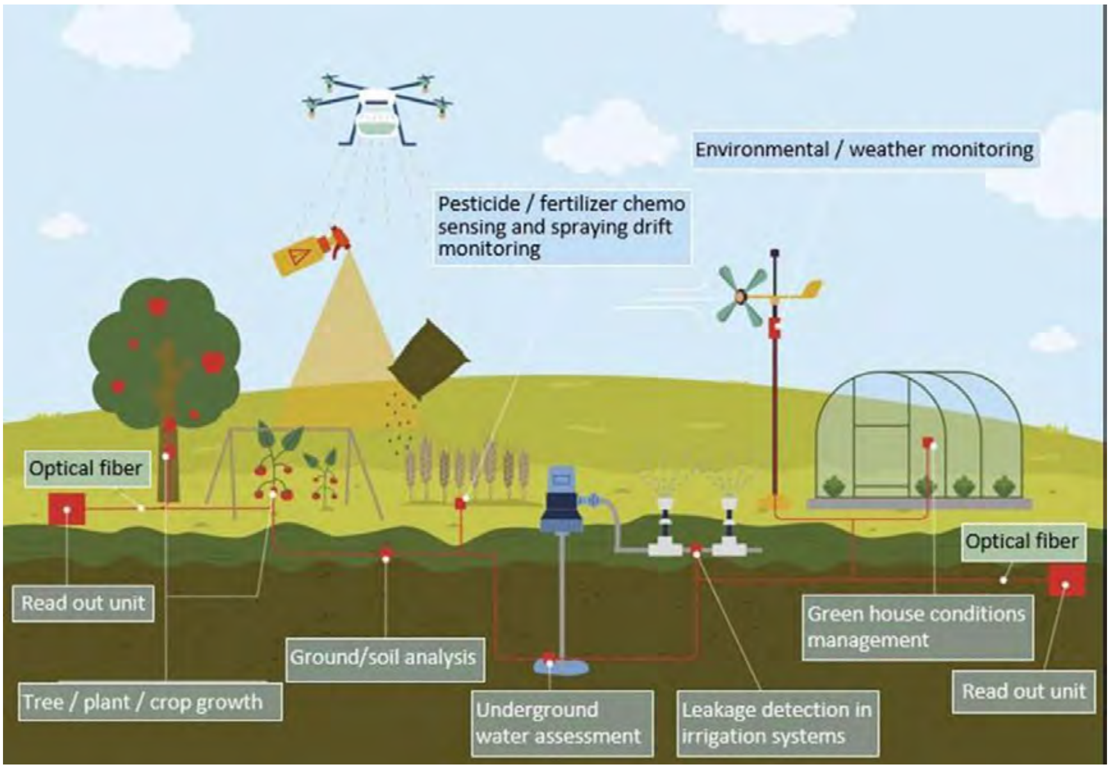

Figure 34. Schematic on existing and emerging applications of optical fiber sensors within the context of precision agriculture.

Concluding remarks

OFSs technology can evolve as a major foundation for the field of PA, prompting its broader adoption by agronomists and farmers, while maximizing the benefits for harvest yield, quality of crops, use of artificial and natural resources, and the environment. It is worthy to say that the plethora of commercialized and experimental OFS devices which already exist can constitute a sound background for their successful implementation in PA applications, minimizing technological risk and development costs, without compromising performance for the endusers. Emerging and future OFSs for PA applications will engage several optical, material, and data processing technologies so to provide new and multi-parametric sensing operations, accessible to non-specialized users, while imparting them with knowledge that would be hard to acquire using standard observation techniques, and the methods currently available. The engagement of diverse technologies into OFSs, will inherently offer them high versatility, allowing them to be applied with small adaptations in open fields, greenhouses, urban farming, or even vertical farming plants, covering the majority of PA cases.

Acknowledgments

Funding by ACTPHAST4.0 EU Horizon2020 Programme, Grant Agreement No. 779472 and LASERLAB-EUROPE, Grant Agreement No. 871124, is acknowledged.

22. Machine learning techniques applied to spectral data

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Status

ML including more recently deep learning, has found extensive applications in the fields of agriculture and food technology [418, 419]. In agriculture some examples include the identification of early signs of crop diseases [420], enabling timely intervention, and reducing crop loss or even animal intrusion [421]. It can aid in optimizing resource allocation by predicting crop yields [422] based on spectral information [423], contributing to more efficient farming practices. In the food industry, ML models applied to spectral data can distinguish between different food types and assess their quality attributes [424], such as freshness, ripeness, adulteration, nutritional content, and chemometric analysis [425]. This technology enhances food safety and quality control processes, ensuring that consumers receive products of the highest standard. Overall, the use of ML on spectral data in food and agriculture empowers stakeholders with valuable insights, enabling them to make data-driven decisions that improve crop yields, product quality, and resource management. Currently used ML techniques include PCA for dimensionality reduction, SVMs for classification tasks, and CNNs to mention only a few.

Unfortunately so far, the applications have primarily focused only on classification [426] and regression tasks [427]. Trained ML models serve as valuable tools, simplifying and expediting specific tasks as described above, however, there is a notable gap in utilizing ML to gain insights into the chemical and physical processes that underlie those events. For example, while ML excels at distinguishing between high and low-quality food products, it has yet to be effectively employed to comprehend the chemical processes responsible for the transformation of a good product into a deteriorated. It is widely acknowledged that ML can be a potent tool for aiding the food and agriculture industries. Nevertheless, the next significant frontier that promises to revolutionize these fields lies in harnessing its capabilities to enhance our understanding of the physico-chemical processes in food production and processing, as well as agricultural production.

Spectral data is the ideal candidate to profit from the power of ML because it contains a large number of specific information it has multi-dimensional information (for example the spectra can be captured under excitation with different wavelengths, in two dimensions as in excitation-emission matrices, or in multiple dimensions, as in HSI) and can be acquired non-destructively, rapidly, and remotely (for example through satellites).

Current and future challenges

As mentioned above, currently the application of ML to spectral data in the field of food technology and agriculture, although extensive, is limited to classification and regression tasks. There is a significant gap in leveraging this technology to gain deeper insights into the intricate chemical and physical processes underlying these events. The major challenges to close this gap can be summarized in six main points (figure 35).

(1) **Extraction of physical and chemical information from spectra**: the development of novel methods, potentially rooted in explainability approaches, is imperative. The methods require the creation of datasets containing spectra paired with informative chemical and physical data, as in [428, 429], which can serve as labels for training ML algorithms.

(2) **Feature selection**: the challenge of feature selection involves identifying relevant spectral bands responsible for or involved in specific physical and chemical processes. Existing feature selection methods have primarily been designed for selecting single features in moderately low-dimensional datasets, such as medical patient information [430]. Adapting these methods for selecting ranges of continuous features, like ranges of wavelengths in spectral data, remains an ongoing challenge.

(3) **Intelligent data processing**: many essential data preparation steps still rely on outdated and inadequate processing algorithms. New approaches, such as generative AI algorithms, have demonstrated remarkable success in tasks like background subtraction and denoising [431, 432], thus warranting adoption for more efficient data processing.

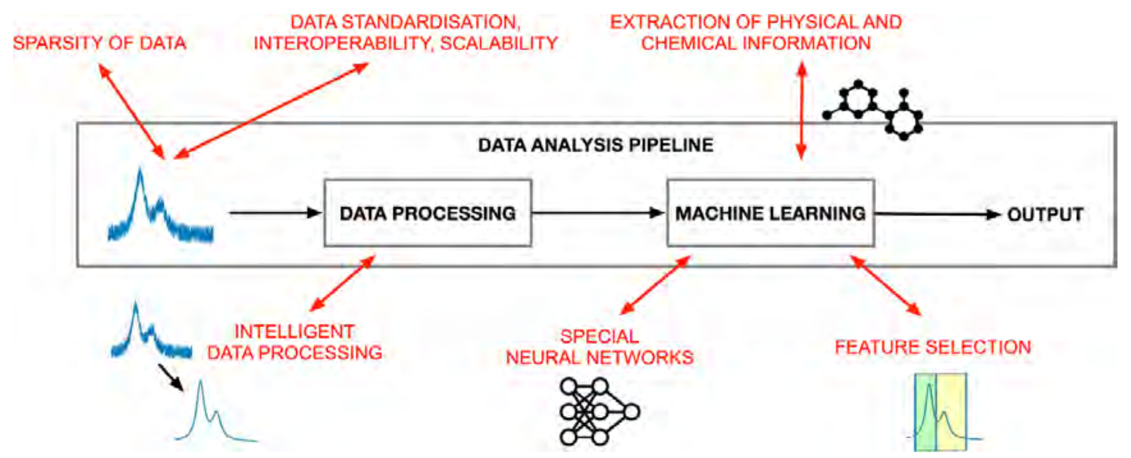

Figure 35. Overview of the major challenges in using machine learning techniques on spectral data.

(4) **Specialized neural network architectures for spectral data**: developing neural network architectures optimized for 1D and 2D data (other than images) is crucial for effective spectral data analysis in food and agriculture. These architectures must be tailored to efficiently process and extract insights from the unique characteristics of spectral data. Current metrics developed in computer vision for 2D images are inadequate for 2D spectral data like excitation-emission matrices.
(5) **Sparsity of data**: the acquisition of a large amount of spectral data always requires time. The datasets are therefore frequently sparse and may be unbalanced for the proper application of ML methods.
(6) **Data standardization, interoperability, and scalability**: ensuring standardized formats and seamless data exchange is essential for integration with agricultural systems, while scalability and efficient processing are needed to manage growing data volumes. Real-time processing is also critical for timely applications like pest detection and quality assessment, requiring advancements in ML/DL algorithm design and system architecture.

In summary, while ML has already contributed substantially to the fields of food technology and agriculture, the formidable challenge lies in expanding its application beyond classification and regression. Leveraging the capabilities of spectral data and addressing the associated challenges in information extraction, data processing, feature selection, and neural network architecture design holds the promise of unlocking deeper insights into the complex chemical and physical processes governing these vital industries.

Advances in science and technology to meet challenges
The advances in science can be classified into six areas.

(1) **Extraction of physical and chemical information from spectra:** explainability approaches have gained traction [428, 429], but they only explain how models (in particular neural networks) work, and are not yet able to explain the underlying physical and chemical processes. Techniques like saliency maps [433, 434], feature selection [435] approaches and SHAP values [436] have great potential but more work is necessary to tailor them to photonics use-cases. Much more work should be done in creating datasets that will enable ML approaches to delve deep into the physical and chemical processes.
(2) **Feature selection**: feature selection in the context of spectral data analysis remains a challenging and evolving area of research. While existing methods excel in selecting single features in moderately low-dimensional datasets (e.g. medical patient information [430]), adapting these techniques to select relevant spectral bands poses ongoing challenges. One promising area of research, especially in the field of spectral data, is the use of genetic algorithms in conjunction with deep learning models to determine the fitness of the proposed band populations [437]. This approach will pave the road to new ways of understanding which spectral bands are relevant for the underlying physical and chemical processes.
(3) **Intelligent data processing**: the field of intelligent data processing has witnessed remarkable advancements, especially in the context of spectral data analysis [438, 439]. Outdated and inadequate processing algorithms could be replaced by more efficient and accurate methods, with generative AI algorithms playing a pivotal role, although those advanced methods have not yet reached the general scientific community, and remain in the status of proof of concepts that are difficult, if not impossible,

to adapt to general use cases. More research on general algorithms that work on a variety of data and spectrum types is still needed to be able for the scientific community to profit from them.

(4) **Specialized neural network architectures for spectral data:** to harness the full potential of spectral data analysis in food and agriculture, specialized neural network architectures optimized for 1D data have emerged as a key focus area [432]. These architectures are designed to efficiently process and extract insights from the unique characteristics of spectral data, such as wavelength patterns and spectral signatures. Researchers are developing tailored models, including 1D-CNNs and recurrent neural networks (RNNs), that can effectively handle spectral data's sequential nature. 1D-CNNs are particularly well-suited for spectral data since they preserve the correlation between adjacent wavelengths through one-dimensional convolutional operations.

(5) **Sparsity of data:** this challenge can be addressed by merging data from multiple sensors and by data augmentation techniques, that can increase the size of datasets synthetically.

(6) **Data standardization, interoperability, and scalability**: establishing unified data standards and adopting open-source, modular frameworks are possible approaches to address this challenge. The realization of efficient data processing allows efficient handling of growing data volumes and the combination of data from multiple sources (data fusion), such as hyperspectral, and conventional imaging, for a more comprehensive analysis of, for example, food quality and crop health.

Concluding remarks

Firstly, the advances in extracting physical and chemical information from spectra have shown promise with explainability approaches. However, there remains a crucial need to develop datasets that enable a deeper understanding of the underlying physical and chemical processes. This would open the road to exploit cross-interferences in the processes to extract more information rather than having to compensate for them. Secondly, intelligent data processing is making incredible strides, with generative AI algorithms poised to revolutionize the field. Nevertheless, these methods are yet to permeate the broader scientific community, necessitating further research to make them widely applicable. Thirdly, feature selection in spectral data remains a challenge. The integration of genetic algorithms with deep learning models offers an exciting avenue for selecting relevant spectral bands, potentially enhancing our comprehension of the underlying processes. Lastly, specialized neural network architectures tailored for 1D spectral data have emerged as a critical focus area. These architectures can efficiently handling the unique characteristics of spectral data, such as wavelength patterns and spectral signatures. In summary, there is still ample room for further research and development in these four areas to fully unlock the potential of spectral data analysis and its applications in various scientific domains.

23. Methods of data classification in spectral studies of food

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Status

Spectrometers, multi- and hyperspectral cameras are examples of photonics devices that have been successfully used in food-related research for many years. The data they produce is described as multidimensional. Often, the first operation performed on the data is to reduce their dimensionality. A popular algorithm in this area is PCA [440–443]. This algorithm facilitates the identification of principal components, which are linear combinations of the original variables and have the highest variance in the data set. This method can be used as a form of preprocessing before the actual data analysis. Dimension reduction reduces this process's computational and memory complexity and avoids over-fitting the model. Reducing the number of dimensions to two or three allows the data to be presented visually, making human analysis possible. In addition to this method, popular approaches are LDA [443, 444], in which linear combinations of variables are found that maximally separate the different classes in the data [445, 446], or independent component analysis (ICA), which is a technique for extracting the independent components of a signal [447, 448].

In the next step, the data are analyzed. Here, a cluster analysis called clustering can be used [449]. This method is used to group similar samples based on the calculated distance between them. There is no single algorithm here that can be called universal. There are many and choosing the right one depends on the characteristics of the data. A simple and computationally efficient one is the kmeans method [441]. It works best when the clusters are spherical and reasonably homogeneous. Another method is hierarchical clustering analysis (HCA) [441, 450]. It is used because it allows the creation of a hierarchy of clusters, which is a tree-like morphology. The data from this analysis can later be presented in the form of a graph called a dendrogram. HCA is divided into two types, agglomerative and divisive clustering. In the first case, there is no need to specify the number of clusters in advance. The process starts with single samples progressively combined with others on the basis of similarity. In the second case, specifying the number of clusters is needed because the process starts with one cluster divided into smaller groups based on internal differences. Among cluster analysis methods, density-based clustering (DBC) [451] or spectral clustering (SC) [452] are also popular in spectroscopy.

Discriminant analysis, factor analysis or regression can also be used to analyze the data. Discriminant analysis is aimed at finding some combination of variables that best separates sample classes. A well-known method is SVMs [443, 444, 453, 454], in which the operation is based on finding hyperplanes that separate different classes of samples in a multidimensional space. It copes well with non-linear relationships between variables. Also worth mentioning is principal component discriminant analysis [445], which combines PCA with discriminant analysis. Factor analysis is a technique that aims to identify the latent factors that make up the observed variables.

Current and future challenges

Supervised methods in AI are playing an increasingly important role in the analysis of multidimensional data. This trend is clearly visible in publications from recent years [455–458]. This also applies to the interpretation of results, which for a long time was left to humans, but now AI is entering this area strongly. When teaching the network today, it is important to ensure that the data are balanced. When they are not, correct classification can be difficult or compromised. Various techniques are used to balance the data, including undersampling, oversampling or weighted cost functions. Although much has already been done, this area is a challenge for the future. The same can be said for methods to reduce the multidimensionality of data. Here, more 'intelligent' methods would be useful, which would be better able to extract information relevant to the study than the current algorithms.

Multidimensional data are often very difficult to interpret, especially the data obtained in the food industry. This is because they reflect complex patterns and relationships that describe the object or compound under study. These relationships can be difficult for humans to detect and subsequently model. High hopes can be placed on deep learning algorithms, which may, in future, be able to deal well with these complex relationships at a more general level. These algorithms are currently being used in spectroscopy, but this relates to specific applications. Graph-based methods, as well as hybrid ones, can be expected to develop.

Another thing that will be a challenge in the future is the scalability of multidimensional data analysis systems. Data sets are becoming larger due to the use of more and more precise and faster instruments [459]. The algorithms that have been used so far may not cope with them, and the challenge will be to develop new, more effective ones.

The use of these techniques in industry is only justified if data acquisition and processing will be realized in real time, looking of course from the point of view of the requirements of a problem under analysis. For example, in nut sorters, where several hundred of them can pass through the device in a second, the acquisition and classification time cannot be longer than a few milliseconds. Such a limitation forces the use of dedicated solutions, where the amount of collected data is limited only to those carrying information about the state of the product, on the basis of which the algorithm that is part of the system can make a quick decision. A challenge in this area is to develop solutions that would be able, based on data from laboratory equipment, to suggest in which bands or wavelengths useful the process information is located and what combination of these bands or wavelengths will give the best results.

Advances in science and technology to meet challenges

The key thing in all research is the quality of the input data. Observing the constant progress in technology, including spectrometry, it can be expected that these instruments will be a source of more accurate and detailed data. More accurate data may allow to better distinguish the individual components of the spectral distribution and their values, which may have a positive impact on better results obtained from data dimensionality reduction or classification methods.

Similar progress is observed in the area of algorithms. It should be taken into account that especially algorithms related to AI will continue to develop very dynamically. These algorithms will be used not only for simple data analysis but the entire measurement and analysis process can be expected to be automated. The algorithms will select optimal parameters for the supervised algorithm and device. This can help both shorten the analysis time and improve the results. Taking the automation path further, we can think about measuring instruments and computing stations in the context of IoT [460]. In this system, locally made measurements would be processed by automated modules specialized in this type of data.

Concluding remarks

Classification methods are a key element of data science. Without them, analysing the data collected by the instruments would be difficult, if not possible. Thanks to their use, it has become possible to widely use complex spectral techniques in the food-related area, among others. The use of AI methods in this area has greatly contributed to increasing the efficiency of classification. The expected further development of instruments and methods, including new classification algorithms, will undoubtedly increase the popularity of this technique and make the data obtained more precise and, therefore, the systems based on them more reliable.

Spectral methods are not only and exclusively spectrometers, multi- and hyperspectral cameras, but also high-speed industrial devices based on selected wavelengths. This area can be expected to develop as the number of food products being inspected increases and as the stages of production at which the inspection is carried out increase. With this growth will come the need to develop more or adapt current classification methods.

Acknowledgment

The Authors would like to acknowledge the financial support of the Institute of Micromechanics and Photonics statutory grant.

Chapter 3: Miniaturization and handheld units

24. Miniature spectrometers, multispectral sensors and the food chain

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Status

In discussing miniature spectrometers, especially in the NIR region, it is important to realize that there is a variety of designs for NIR spectrometers, used for different purposes [461]. Specifically, the main traditional NIR applications are in food, feed and agriculture [462], and many of these are ***quantitative***, the result of many years accumulation of data, careful instrument and sampling optimization, and are used for transactional and quality applications. As a result, migrating those applications to a miniature or portable spectrometer are unlikely, though newer semi-quantitative applications can be developed. A second large application area is ***qualitative***, especially material identification and related areas (detection of contamination or counterfeit materials, etc) [463]. Many of these applications fall into the category of 'screening in the field' and are therefore amenable to the use of portable spectrometers. The third major area is process monitoring and analysis [464], where many other considerations come into play, including ability to operate in hazardous areas, long term stability, insensitivity to vibration, temperature and humidity changes, fiber optic interfaces, etc.

Portable spectroscopic instruments [465], in general, do not have spectroscopic performance of lab instruments, but are optimized for use in the field by non-specialists. However, they are ruggedized, often come with built-in or cloud-based qualitative and new quantitative applications, and provide instant answers at the point of need. A wide variety of technologies are used, with newer generations of these instruments becoming ever smaller [466, 467]. There are performance trade-offs with size reduction (spectral range, spectral resolution and signal-to-noise), and so a judgment has to be made as to whether the performance is 'good enough' for a particular application (figure 36). Attention also has to be paid to the sampling interface [468] to ensure that quality spectra are obtained, for instance from a representative sample, with minimal stray light, etc. In many cases, these instruments can operate in 'point-and-shoot' mode [469], i.e. they do not require a sample to be handled or prepared in any way and can possibly be interrogated by optical spectroscopy inside a glass bottle or plastic envelope.

Further advances include continuing miniaturization, the use of smartphone interfaces [470], applications of data processing in the cloud, and newer photonic approaches. These approaches may enable the manufacture of significantly lower cost instruments, leading to their wider use and development of new application areas [471]. Two significant areas are the emergence of very low-cost multispectral sensors [472, 473] and planar geometry PICs (also known as silicon photonics) [474].

Current and future challenges

Two challenges stand out: the technologies to miniaturize and cost-reduce spectrometers further (described below), and the development of ***applications*** to deliver actionable answers to the operator, and not just spectra (figure 37).

Identification or classification (i.e. what group does this belong to) of a material is qualitative analysis [475]. The spectra of pure materials, or those which are identified by a brand name (and likely to be homogeneous), are compared with spectra in a database (a spectral library). The library should include spectra of all the substances that might be found in that environment, and not just the ideal analytes. The main application effort involves acquisition of well-characterized, genuine, samples, running their spectra, and building a library or calibration. For a specific application, a careful choice of instrument may be required, depending on the system under investigation.

Determining the concentrations of components of mixtures is quantitative analysis. However, optical spectroscopy, while rapid and convenient, is a secondary or indirect technique. Models have to be built based on samples that have been analyzed by a primary or reference technique [476]. These established methods, can be time-consuming and expensive. Those results, and their spectra are combined in a chemometric method. Validation samples, similarly analyzed, need to confirm that the model works appropriately, and is not using 'accidental' correlations.

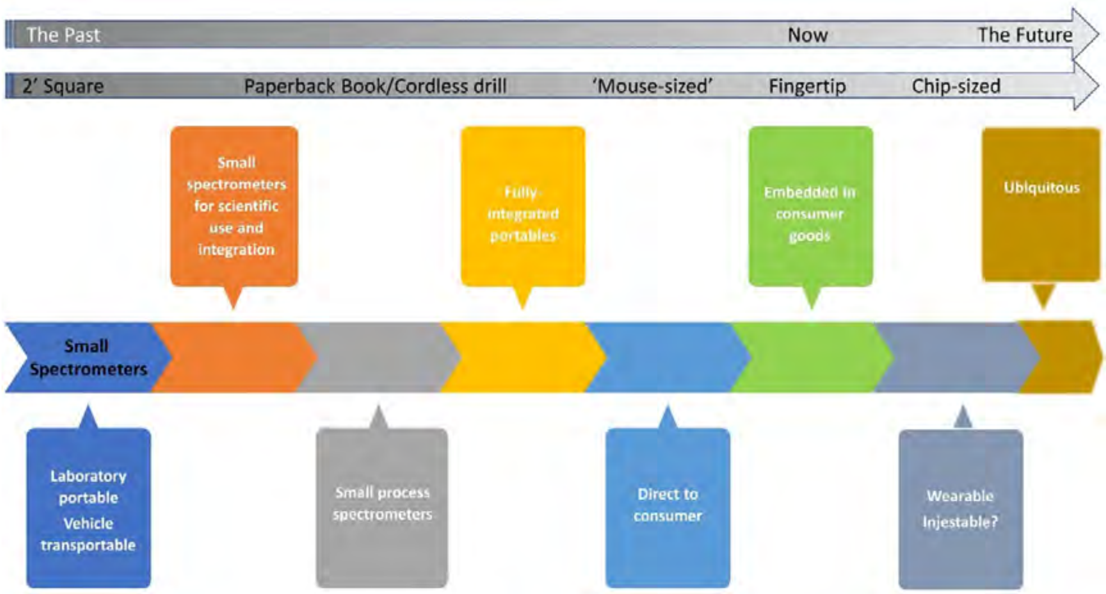

Figure 36. The trend for ever-smaller spectrometers, and their possible application areas.

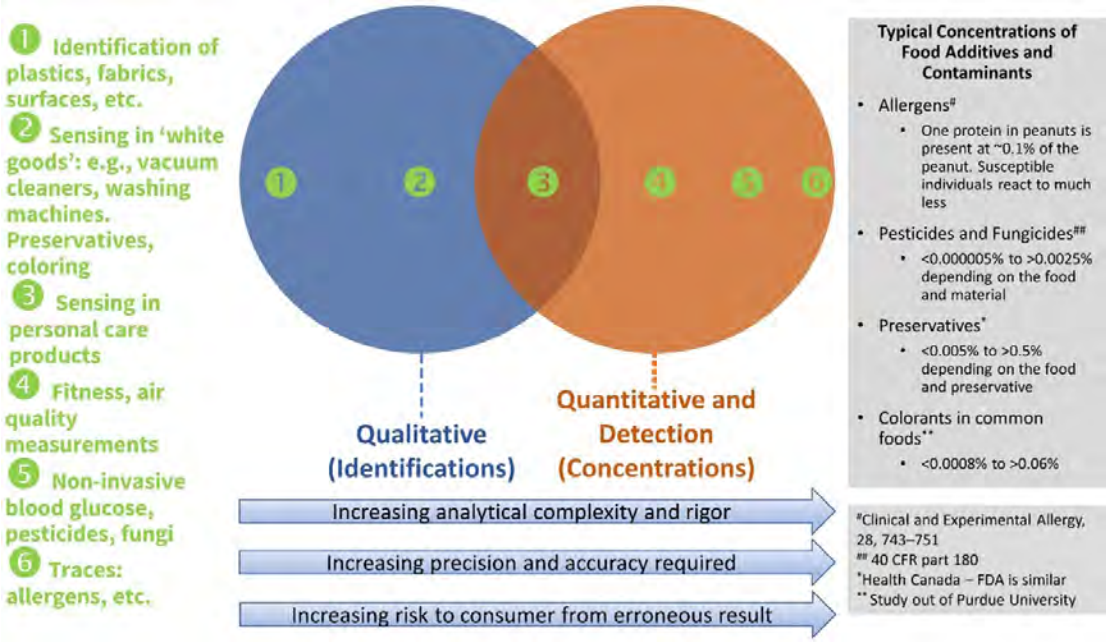

Figure 37. Miniature spectroscopic devices may be used for qualitative, detection and quantitative applications. The complexity of the analysis, and its required precision and accuracy, increase from qualitative to quantitative applications, and so does the risk to the operator and consumer if an erroneous result is given.

Many of the new miniature spectroscopic technologies come from groups who are not analytical spectroscopists, and are not aware of these challenges, which has led to some exaggerated claims being made. One concern is that some of the new vendors propose to use 'crowd-sourced' data. This raises two questions: the quality of the spectroscopic measurement, and the accuracy of the identification, and/or quantitative information, usually referred to as 'metadata. In addition, improper presentation of the specimen to the spectrometer can lead to stray light errors, invalidating quantitative methods. Finally, small instruments typically interrogate small specimen areas, which is problematic for heterogeneous samples [468]. There is real danger of 'garbage-in, garbage-out', with these approaches. A second possible concern is with some vendors where there also seems to be a lack of understanding about detection limits of optical spectroscopy in the condensed phase. This leads to claims of detecting trace amounts of allergens, pathogens, pesticide or herbicide residues (figure 37). It is generally accepted that with condensed-phase optical spectroscopy, detection limits are in the low percent range, absent any separation or enhancement techniques.

Advances in science and technology to meet challenges

The latest development in portable spectroscopy is the availability of very low-cost multispectral sensors, the size of computer chips [477]. The width of absorption bands in the VNIR regions for condensed phase samples imply that an instrument with a small number of resolution elements will be able to perform routine analyses, and that spectral range is a more important parameter than spectral resolution. Multispectral devices can be produced in volume via semiconductor and optical coating techniques, at very low cost—less than $10 each. Here we are defining a multispectral sensor as a device observing a small number of spectral bands (around 8–16), at broad resolution (around 20–50 nm). An example of a low cost (disposable) device in the agricultural area is a multispectral sensor designed to be inserted into an immature bunch of grapes, growing on the vine, to monitor their maturity [478].

The ideal next step would be for all the photonic components, including the electrical contacts required to drive them, to be integrated onto a wafer, and produced *en masse* using semiconductor manufacturing techniques. This is the promise of silicon photonics and PICs, and research in this area has been ongoing for more than twenty years, with roadmaps laid out for the future. The vision is similar to integrated circuits replacing discrete transistors and other electronic components, enabling mass production of highly integrated chips. A key point here is that conventional spectrometer designs (dispersive, Hadamard, FT) result in approximately cubic form factors; much of the research and development coming from the electrical engineering and semiconductor communities is focused on silicon photonic planar structures, which could enable facile integration with small consumer products like smartphones and smart watches.

The economic driver for much of this activity is the field of consumer 'wearables': health monitors, rings and patches. A typical ring contains multiple sensors: red and green LEDs, thermal coefficient body temperature, a 3D accelerometer, and a gyroscope. The annual unit volumes for these consumer devices are potentially in the hundreds of millions, with revenues around $30 billion, which has driven down the cost of photonic devices (such as vertical-cavity surface-emitting lasers—VCSELs—for facial recognition) dramatically. The same could happen soon for visible-NIR multispectral or Raman-based sensors.

Concluding remarks

With further miniaturization of optical spectrometers, and their concomitant cost reduction, a number of natural products and food applications become commercially feasible. A large demand for cannabis analysis has emerged following the legalization of cannabis in Canada (among other places), and of hemp in the USA. As noted above, pesticide and herbicide residue analysis require a laboratory technique, but with appropriate calibrations in place, routine analysis of bulk components can be done with a portable optical technique.

New instruments and applications in food, feed and agriculture are appearing, given the increasing emphasis on PA. For instance, a portable NIR spectrometer, with an integrating sphere sample interface, can analyze protein, moisture, carbohydrates and oil content from crops [479], and a soil nutrient scanner [480] is also commercially available. In both the USA and Europe there have been initiatives for food assurance, using broadband visible-NIR spectroscopy, combined with the necessary reference analyses, to categorize produce for quality. One approach is to provide customers with information about the quality of produce in the store, and working with grocery retailers to improve that quality. Detection of food hazards, spoilage and food fraud is a second.

25. Ultra-miniaturized spectrometers and their agro-food applications

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Status

In pursuit of PA, there is a great need for the development of optical technologies to monitor crop health and soil conditions. Optical spectroscopy is one of the most effective approaches for these purposes (e.g. to detect signs of fertilizer deficiency or excess well before visual symptoms appear on the plant). This can enable farmers to optimize the distribution of water and fertilizers, grow plants with resistance to diseases and pests, and increase the quantity and quality of their crops. Currently, such plant diagnosis is carried out by taking leaves off plants and measuring their spectral signatures in laboratory settings. For non-invasive on-site inspection, crucial requirements for the widespread adoption of these technologies, it is necessary to drastically decrease the size, weight, and cost of optical spectrometers. Recently, a new class of ultra-miniaturized reconstructive spectrometers has arisen that promises to address these issues.

Conventional spectrometers rely on bulk optical components to separate colors from one another for detection, and therefore cannot be miniaturized without sacrificing performance. The spectral resolution of grating spectrometers (figure 38(a)), which to date remain the gold standard for bench-top systems, generally speaking scales with linear dimensions. Spectrometers using a series of narrow-band spectral filters to isolate individual colors for detection are relatively smaller in size (figure 38(b)); their spectral resolution is determined by the linewidth of each filter, which can be deeply sub-nm even for miniaturized filters, but their operating bandwidth—that is, the number of filters—scales with the device footprint, and it is not practical to have more than a few tens of filters [481]. To further reduce the device footprint, a single tuneable filter can be used, but at the expense of measurement speed [482].

Reconstructive spectrometers overcome these trade-offs by not requiring that colors be completely separated from one another for detection. Instead, they are designed such that each input wavelength produces a complex but unique pattern in the output signal. For example, spectral information can be extracted from the complex way in which light scatters in a random medium [483], or from the patterns of light leaking from a multimode fiber taper [484–486]. These devices harness multimode interference to create wavelength-dependent spatial distributions, with interference regions of just a few hundred microns in length being sufficient to obtain pm-level spectral resolution. However, external optics and detectors are required to read the spatial patterns, hampering the portability of these spectrometers.

'Ultra-miniaturized' spectrometers combine the spectral sensitivity and the photodetection in a single component element [487], for example by modulating the spectral response of an electrical junction (figure 38(c)) [466]. If the responsivity of the device is known, the spectral content of unknown input light can be reconstructed from the variations in photocurrent as the applied electrical voltage is swept. Nanometer-level spectral resolutions are possible even though the total footprint of the device is on the order of a few tens of micrometers. Bringing such ultra-miniaturized spectrometers to the field would be of enormous benefit for agriculture and the food chain.

Figure 38 shows a comparison of the working principles of conventional spectrometers (i.e. a grating spectrometer and a filter-based spectrometer) with that of an ultra-miniaturized reconstructive spectrometer.

Current and future challenges

The working principle of ultra-miniaturized reconstructive spectrometers relies on the ability to tune the wavelength dependence of the responsivity of a photodetector. Broadly speaking, we can separate these devices into two categories (i.e. bandgap and interface modulation, table 2), based on the tuning method used. Some implementations tune the bandgap of a single active material (e.g. via the Stark effect [488], or by varying the composition of compound semiconductors [489, 490], or through the application of strain [491]) while others electrically modulate the energy barrier height in a junction between two materials (such as between MoS_2 and WSe_2 [492], MoS_2 and Black Phosphorous [493], or ReS_2 and WSe_2 [494]). After characterizing the response of the device to a series of known spectra (typically, monochromatic illumination is used), it is possible to infer the frequency content of unknown spectra by analysing the device's output using a computational algorithm [495]. With a sufficiently dense training dataset, and if the modulation is strong enough (meaning if there is enough change in the responsivity of the device as a function of wavelength as the applied voltage is varied) performance comparable to table-top spectrometers is possible,

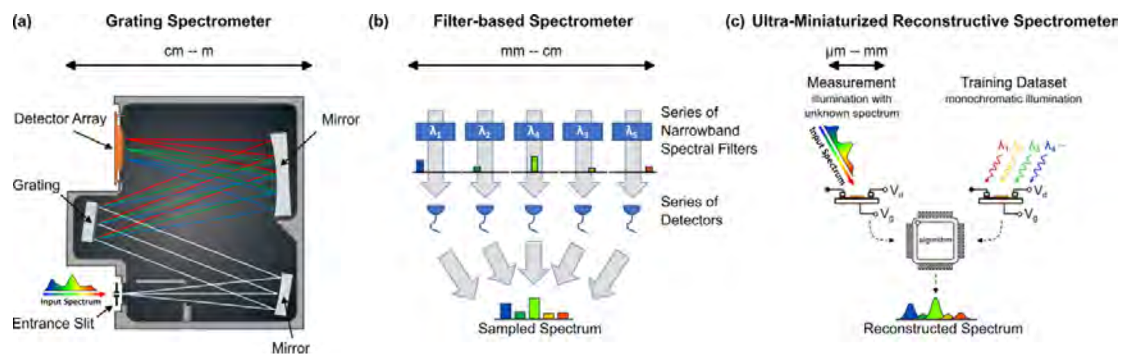

Figure 38. Comparison of working principles of a grating spectrometer, a filter-based spectrometer, and an ultra-miniaturized reconstructive spectrometer based on modulation of an electrical junction.

Table 2. Performance comparison of ultra-miniaturized reconstructive spectrometers reported in literature.

Working principle	Material	Spectral range (nm)	Spectral resolution	Size	References
Conventional	Table-top grating spectrometer	500–1000 VIS	<0.1 nm	600 × 350 mm^2	Typical values from references of [466]
	Portable grating spectrometer	200–1050 VIS	0.5–12 nm	90 x 60 mm^2	
Bandgap modulation	Nanowire (Silicon)	450–800 VIS	6 nm	2 × 2 mm^2	[487]
	Nanowire (CdS_xSe_{1-x})	500–630 VIS	10 nm	75 × 0.5 μm^2	[489]
	Black phosphorus	2000–9000 MIR	40 nm	16 × 9 μm^2	[488]
	MoS_2 (Strain)	400–860 VIS	1.2 nm	20 × 25 μm^2	[491]
	III–V semiconductor	480–820 VIS	10 nm	20–500 μm Ø	[496]
	Perovskites ($KMAPbCl_xBe_{3-x}$)	450–780 VIS	80 nm	5.6 × 5.6 μm^2	[490]
Interface modulation	MoS_2/WSe_2	405–845 VIS	3 nm	22 × 8 μm^2	[492]
	MoS_2/Black Phosphorous	500–1600 VIS/NIR	2 nm	30 × 20 μm^2	[493]
	$ReS_2/Au/WSe_2$	1150–1470 NIR	20 nm	6 × 4 μm^2	[494]

even though the reported active footprint of these nanomaterials-based reconstructive spectrometers is of the order of mm^2 or less.

Although ultra-miniaturized reconstructive spectrometers have been demonstrated to work well in a laboratory setting, there are fundamental challenges that need to be addressed before they can be deployed to the field. First, since their performance is primarily based on bandgap or interfacial barrier modulation, they normally function over a limited spectral bandwidth (table 2). Second, the nanoscale materials used in their construction are typically grown at laboratory scale, and most of them are not yet developed industrially. Thus, the industrial adoption and mass-manufacturability of these ultra-miniaturized spectrometers is a serious challenge. Third, some of the nanoscale materials are unstable in ambient environments, which leads to significant device-to-device variation and calibration issues. For the reconstruction algorithm to work, it is important that the spectral responsivity remain constant between the training and measurement steps. Therefore, the stability and robustness in on-field operating conditions with changing temperature and humidity are a critical issue.

Advances in science and technology to meet challenges

There has already been some progress to mitigate these challenges at the laboratory and industrial level. While improvements in materials processing technology have enabled some nanoscale materials like graphene to be grown at large scale by chemical vapor deposition—in fact, wafer-scale growth of graphene is nowadays offered as a foundry service—the fabrication of 2D material heterostructures remains a laborious manual task. Recently, there has been some progress in developing semi-automatic systems to assemble van der Waals heterostructures [497] but not at industrial levels. Therefore, there is great interest in realizing ultra-miniaturized spectrometers based on scalable materials such as silicon, compound semiconductors, and organic materials, which can reduce the lab-to-fab duration for such technologies. A III–V semiconductor-based reconstructive spectrometer was recently reported [496], proving a promising approach for massively parallelized fabrication. A fully-CMOS-compatible design would enable us to leverage the mature silicon electronics manufacturing and design ecosystem and manufacture such spectrometers at industrial scale.

The stability of these devices could be improved with adequate surface passivation. For example, alumina encapsulation by atomic layer deposition has been shown to improve the stability of perovskites in aqueous environments [498]. Alternatively, ultra-transparent glass encapsulation can be used to shield the device from the environment without loss of performance [499]. Additionally, routine on-site calibration against a reference sample can be employed to realize stable device performance.

Significant research effort is also being put towards the improvement of the reconstruction algorithms, with an emphasis on robustness to noise. As the amount of noise that can be tolerated by the algorithm increases, the required signal-to-noise ratio decreases, thereby allowing for faster data acquisition with shorter integration times. Currently, most implementations of reconstructive spectrometers use regularization/minimization algorithms. Generally, for reconstruction algorithms, a large dataset is needed for learning purpose to establish relationships between the measurements and the reconstructed algorithm (sampling). This makes the calibration process slow. However, adapting deep learning and neural network models can mitigate this issue to some extent. There is some indication that ML models can outperform regularization in the presence of noise, but more research on this field is necessary. This issue requires interdisciplinary and collaborative approach among researchers of different domains.

Concluding remarks

Ultra-miniaturized reconstructive spectrometers are an active field of research that pushes the miniaturization of spectrometers to its limit. The initial laboratory results have shown great prospects in terms of performance, paving way for possible applications in PA. As can be seen in table 2, there is a great variety in material platforms among the reported devices, allowing researchers and farmers to choose the working bandwidth according to the requirements of their specific application, e.g. signatures of nitrogen deficiency can be detected in the fingerprint spectral region (7–14 μm). These spectrometers tend to be lightweight, and therefore are the ideal choice for integration with transport media (hand-held devices, drones, satellites etc), where they are expected to offer significantly reduced payload compared to conventional spectrometers for practical on-site or remote inspection. For many of the designs listed in table 2, voltages $<$5 V are required for operation, and with modest power requirements, it should be possible to drive these devices with on-board electronics. If CMOS compatible designs are developed, the readout circuitry can be directly built in the sensor. Furthermore, arrays of such spectrometers could be used to implement HSI in a compact form factor.

Acknowledgments

This work was supported by Business Finland (R2B A-gate), Academy of Finland (314810, 333982, 336144, 352780, 352930, 353364, 359009, 365686 and 360411), the Academy of Finland Flagship Programme (320167, PREIN), the EU H2020-MSCA-RISE-872049 (IPN-Bio), the Jane and Aatos Erkko foundation and the Technology Industries of Finland centennial foundation (Future Makers 2022), and ERC (834742).

26. Portable biophotonic systems for agro-food analysis

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Status

Currently, the majority of tools for food quality control during the collection and processing of raw materials, as well as during the production of food products are still based on heavy analytical methods which provide a strict quality control but are complex, expensive, time-consuming with time-to-result up to several days, and applicable in laboratory environments.

Chemical analysis techniques such as chromatography (e.g. gas chromatography, LC) [500] are widely used for detecting contaminants, pesticide residues, and food additives. Those techniques require expensive equipment and are reliant on timely procedures which involve highly skilled personnel [501]. For detecting foodborne pathogens, culturing and plating assays are considered the gold standard [502]. However, these methods are also considered demanding and slow procedures, often taking several hours to days to yield results. ELISA method is able to address this challenge as offers a much faster detection [503], however it is less specific compared to other methods and involves multiple processing steps. Similarly, PCR method, also required multiple steps, including nucleic acid extraction, amplification, and detection [503].

Conversely, biosensor devices, both for traditional as well as PA [504], are analytical devices that can provide quantitative analysis, thus covering a large part of the distance between the functionality of the analytical methods and that of low-cost screening toolkits. Additionally, biosensors can also be made portable, designed to be more user-friendly, disposable, and manufactured at a reduced expense. Up to date, different biosensor platforms have been the focus of interest including fluorescence-based [505], electrochemical [506] and surface acoustic waves-based [507]. However, and despite their individual strengths, these platforms still have individual limitations such as need for labeling [508], need for utilization of bulky setups, in many cases involve time-consuming multistep detection protocols while also present low signal-to-noise ratio. A novel category of biosensors is made possible by controlling the interaction between light and matter. Photonic biosensors can be collectively fabricated, making the manufacturing process more efficient and cost-effective, enable the simultaneous detection of multiple analytes, present high sensitivity while also are less susceptible to electromagnetic interference or noise, making them suitable for use in various environments, including those with electromagnetic interference. Furthermore, the optical biosensors enable the real-time and label-free detection, thus simplifying experimental procedures and reducing potential artifacts. Photonic biosensors base their operating principle either in the interaction of the escaping evanescent wave, as the light propagates on the waveguide, with the desired analyte, or by directly exploiting the optical properties of the analyte (spectroscopic biosensors). For the evanescent-based biosensors, figure 39 illustrates a representative example of a fully integrated Lab on Chip (LoC) device utilizing such sensors. Based on the operating principle, a bioreceptor molecule is immobilized on the surface of a waveguide and upon interaction with a bioanalyte, a variation of the signal is obtained at the output of the device. The evanescent wave has an interaction field with the analyte in the nm scale, thus it is protected from occurrences within the main body of the sample [509] and as a result, photonic biosensors exhibit high sensitivity [510]. In the field of food quality monitoring photonic biosensors have already been used for the detection of pathogens and pesticides drugs and chemicals in food samples [511] or water [512].

Current and future challenges

Several challenges must be addressed so as to exploit the full potential of such sensors. The **sensitivity of the sensors mostly** depends on the choice of biorecognition elements. Antibodies, are the most common elements, having demonstrated their ability for high sensitivity (low detection limits) in various types of biosensors [514]. **Specificity** issues that all types of label-free biosensors still face today are related to their biochemical part. It is common to have a system capable of detecting an analyte with high sensitivity, but at the same time not being able to distinguish between this analyte and closely related biomolecules, mainly due to the fouling effects from these other molecules that are present in real-life complex matrices [515]. **Compactness:** despite the impressive progress on photonic integration on PICs devices [516], the compactness of the photonic part of the sensors is still limited, as in most cases the optical sources and the detection elements are placed off-chip and are connected with the photonic chip through external optical couplers. **Sample handling:** the PIC biosensor devices are integrated onto a final LoC device with the use of

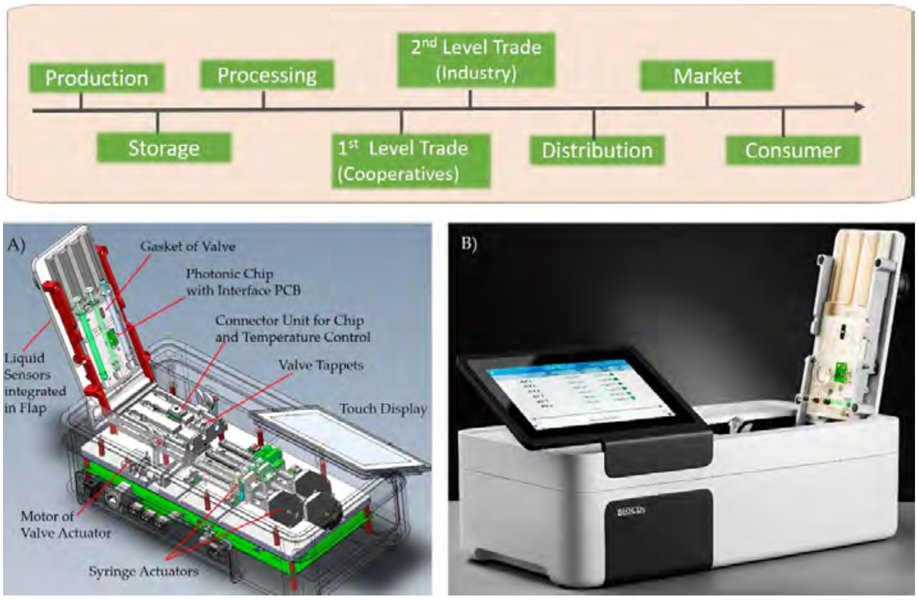

Figure 39. Top: agrofood chain from farm to fork. Bottom: an example of a LoC device with integrated photonic sensor (A): BIOCDx photonic biosensor device with inserted cartridge, (A) 3D model, and (B) final instrument. Figure reproduced from. Reproduced from [513].

microfluidic cartridges that are able to perform the sampling, sample treatment, sample concentration and sample delivery onto the sensor surface [513]. There are several challenges associated with the use of such microfluidic chips that limit the advantages of the PIC biosensors. Although photonic biosensors are known for their fast response time, the use of such fluidic cartridges often lead to longer detection times [517]. Additionally, even though the use of microfluidic cartridges enables the development of a disposable sensor devices, often come with the need for bulky and expensive external microfluidic peripherals [509]. **Low cost:** the development of ultra low-cost, disposable devices has been the dominant model for the development and commercialization of all types of LoC platforms so far. This approach is used to avoid cross-contamination issues and complicated cleaning protocols associated with biological samples. However, the single-cartridge use approach often involves the use of biomaterials and chemical reagents related to the functionalization of the photonic sensors which, often increase the cost of the cartridges drastically [518]. There are also other challenges such as field testing and validation, regulatory compliance, standardization, market awareness and adoption that should be mentioned but are not discussed here.

Advances in science and technology to meet challenges

Regarding the scientific and technological challenges described above, improvements have been and are being made, to address those issues. Concerning the **sensitivity** of the biorecognition elements, there has been an increased use of aptamers since their smaller size can achieve high sensitivity due to the higher density surface coverage with more available binding sites per surface area. As far as the **sensitivity** of the chip-integrated waveguide sensors in recent years, the waveguide sensitivity has been improved by combining the MRRs with slot-waveguides or subwavelength grating (SWG) waveguides. Relating to the **selectivity/specificity** of the sensing mechanism, through ongoing efforts in recent years, certain label-free optical transducers have made significant strides, allowing them to accomplish the detection in complex matrices [519] of individual molecules such as by the formation of a hydration layer with hydrophilic compounds [520] or the formation of an effective charge-balanced layer with zwitterionic compounds [521]. Also, polymeric flow-through microfluidics can be used for improved response time and selectivity [522]. Concerning **compactness**, significant effort was made to alter the integration method by incorporating both active and passive optoelectronic components, along with the electronics layer, onto a single sensor chip. Moreover, the evolution in optical biosensor innovation is characterized by the incorporation of nanophotonic biosensors [510], which can achieve significantly enhanced miniaturization, portability, and throughput. Another significant challenge, is the chip packaging with microfluidics and electronic readout connections. A novel integration approach to overcome this issue was introduced in 2020 [523] whereby a local backside-release process to separate the electronics and optics from the microfluidics has been developed. In addition, an approach utilizing integrated digital microfluidics [524] can further increase the portability of the system. Regarding **low cost and reusability**, nowadays, other biorecognition elements are being used such as aptamers especially DNA-based ones, which offer the possibility to fabricate biosensors that are reusable over many cycles. Furthermore, **low-cost** methods manufacturing microfluidic chips via digital light processing (DLP) or grayscale DLP can further reduce overall system cost while also there is a tendency to introduce smartphones in the novel biosensor devices, thus exploiting the light sources, cameras, image processing and communication capabilities [525].

Concluding remarks

The need for effective screening tools that will be fast, low-cost, sensitive, truly reliable and portable for use at food production sites and processing units, is here and is urgent. However, as with any new approach there are several challenges that need to be addressed. Overcoming these challenges requires a multidisciplinary approach involving scientists, engineers, policymakers, and industry stakeholders. Continuous innovation and investment in biosensor technology will play a significant role in addressing the unique challenges of the agri-food industry and ensuring a safer and more sustainable food supply.

Acknowledgment

This project has received funding from the European Union's Horizon Europe Framework Programme research and innovation action under Grant Agreement No. '101093150'.

27. Lab-on-a-chip (LoC) systems for agriculture

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Status

Growing awareness for environmental protection and sustainability, coupled with limited land and energy resources and the impact of climate change, are placing increasing demands on agriculture and food production. To meet these challenges successfully and to address the trade-offs between sustainability, productivity and food/feed quality, optimized processes and new technologies are essential [526, 527].

The use of analytical technologies in agricultural processes as an enabler for precision farming offers many opportunities [527]. Analytical technologies are particularly relevant for

- **Monitoring the agricultural and aquacultural environment** to ensure optimal conditions for growing plants or animals (e.g. soil moisture, pH level, nutrient content) [528].
- **Monitoring the quality or safety of food and feed** (e.g. detection of pests like pathogens and micro-organisms).

Current analytical technologies use electrochemical, optical, colorimetric, and biological methods. As these techniques are typically applied in specialized laboratories, they have the following **disadvantages** [529, 530]:

- initial costs are high
- the equipment requires space and lab infrastructure
- trained professionals are needed for operation
- tests cannot be performed on site and samples need to be transported to the laboratory. Analysis is therefore time-consuming and action cannot be taken immediately.

For time urgent and precise decision making new sensing technologies are needed:

Microfluidic LoC systems typically consist of a readout device operated with exchangeable analytic LoCs (figure 40). They integrate multiple functions for characterization of liquid samples onto a single platform, enabling faster analytical testing with precision comparable to specialized labs. These systems offer several **advantages**:

- portability
- cost effectiveness
- the ability to provide real-time data
- enable farmers to make informed decisions at the point of need.

One prominent application is soil health monitoring. Additionally to traditional methods of measuring soil pH and moisture levels, LoC systems can e.g. analyze nutrient content accurately, allowing farmers to tailor their fertilization and irrigation practices, thereby optimizing crop yields while reducing resource wastage [531].

Water quality assessment is another vital area where LoC systems can make a difference. They enable the analysis of water sources for contaminants such as heavy metals, pesticides, and pathogens. This is crucial for ensuring crop safety and preventing environmental pollution [527].

Moreover, LoC systems can be employed for rapid pest and disease detection. By analysing plant samples, these systems can identify pathogens or pests quickly, enabling farmers to take timely action, such as targeted pesticide application or crop removal, to prevent further spread [532].

Current and Future challenges

However, there are also challenges in using LoC technology in agriculture (table 3):

Fabrication and cost of LoCs: LoCs require precise and complex fabrication techniques, such as microfluidics, nanotechnology, and biotechnology, which can be expensive and time-consuming. Moreover, the materials used for LoC systems should be biocompatible, durable, and scalable, which can limit the choice and availability of suitable materials. Therefore, there is a need to develop low-cost, simple, and robust fabrication methods and materials for LoCs that can be mass-produced and widely distributed [533].

Figure 40. Lab-on-a-Foil (®JOANNEUM RESEARCH).

Table 3. Summary challenges and technology advances.

	Current and future challenges	Advances in Science & Technology
Fabrication and cost	Mass production is expensive, time consuming and difficult to scale	Continuous roll-to-roll manufacturing
Biobased and biodegradable	Non-renewable resources used for single use components	Adoption of recycled or bio-derived materials
Integration and Automation	Complex sample preparation and analysis in a centralized lab	Microfluidic Lab-on-a-Chip (LoC) systems integrating all required functions at the Point of Need
Sensitivity and specificity	Detect and quantify low levels of target analytes, in complex and heterogeneous samples	Translating innovative biosensor approaches initially developed for human disease diagnostics
Standardization and regulation	Lab-on-a-Chip (LoC) systems should comply with relevant standards and regulations	Adoption and support from governmental regulations can drive implementation of LoC
Throughput	Increase throughput for more efficient and sustainable agricultural practices	Miniaturization of analytical processes, enabling (parallel) on-site testing without trained personnel.

Biobased and biodegradable: most LoC systems are currently single use, made from plastic materials derived from non-renewable sources and ending as medical/diagnostic waste in landfill. To move towards a circular economy, reduce the overall carbon footprint and commit to net zero, it is necessary to look at the entire product life cycle. This includes the development of new biodegradable materials, also from natural sources, taking into account their own environmental issues. More generally, the LoC field needs to address key challenges related to global sustainability goals, reducing single-use plastics in analysis and using low power, recyclable microsystems technologies [534].

Integration and automation: there is a continued need to move analytical tests away from specialized and centralized laboratories and into community settings to enable operators to make informed decisions at the point of need. Required are smart and adaptive LoC systems that can integrate and automate various functions in a chip/device [535].

Sensitivity and specificity: LoC systems should be able to detect and quantify low levels of target analytes, in complex and heterogeneous samples, such as food, water, soil, and biological fluids. This can be challenging due to the presence of interfering substances and the variability of environmental conditions. This results in the need for sensitive and specific LoC systems that can enhance the signal-to-noise ratio, reduce the

Figure 41. Roll-to-roll (R2R) pilotplant for UV nanoimprint lithography of microfluidic structures, microarray spotting of biomolecules and UV-lamination (®JOANNEUM RESEARCH).

false-positive and false-negative rates, and increase the accuracy and precision of the detection and analysis [535].

Standardization and regulation: LoC systems should comply with the standards and regulations of the food, agriculture, and biosystems industries, which can vary depending on the country, region and application.

Throughput: improving the throughput of LoC systems is essential for enhancing their application in agriculture. Overcoming current constraints will enable faster diagnostics, large-scale monitoring, and better integration with automated systems, ultimately supporting more efficient, sustainable agricultural practices and timely decision-making in precision farming [536].

Advances in science and technology to meet challenges

Looking forward, the future of LoC technology in agriculture seems promising. Continued research and development efforts, coupled with advancements in nanotechnology and microfluidics, are expected to enhance the performance and reliability of these LoC systems.

Fabrication and cost of LoCs: Roll-to-roll (R2R) imprinting technology facilitates efficient, high-throughput fabrication of micro- and nano-structures over large areas. The process uses flexible polymer foils, allowing for subsequent modifications such as bio-functionalization, hole cutting, or chip lamination, all within the R2R manufacturing framework. In an R2R UV-nanoimprint lithography (UV-NIL) process, structures are replicated from a polymer, nickel, or steel master (referred to as a 'shim') onto an uncured photoresin layer applied to a polymer substrate (figure 41). The photoresin is cured under UV light while in contact with the shim, forming solid microfluidic structures on the foil. This process takes place at room temperature, under low pressure, and in ambient air conditions, enabling the creation of precise microfluidic features such as V-grooves or rectangular channels. The method holds considerable potential for scaling up production and reducing costs for LoC systems. Overall, R2R imprinting offers an industrially efficient solution by reducing manufacturing costs, resource usage, and energy consumption, while enhancing production throughput for micro- and nano-structured devices. [533, 537, 538].

Biobased and biodegradable: adopting recycled or bio-derived materials for single-use LoC components can reduce CO_2 emissions and plastic pollution. Material choice must consider manufacturing and disposal processes [539]. Despite slow progress, the potential for circularity is emerging, with over 130 European bioplastics projects conducted between 2007 and 2020 [540].

Integration and automation: LoC systems often involve multiple steps and components, such as pumps, valves, sensors, actuators, and microcontrollers, which are integrated on a single chip. This involves new designs for different assays and consideration of compatibility, reliability, and functionality of the LoC systems. Moreover, development of LoC systems includes automated and autonomous sample preparation [541, 542].

Sensitivity and specificity: there is great scope for translating innovative biosensor approaches, initially developed for human disease diagnostics, to the early detection of plant pathogens. Especially electrochemical and optical biosensors may provide innovative solutions for plant pathogen detection and management in the future [532].

Standardization and regulation: increased adoption and support from agricultural institutions as well as governmental regulations can drive the implementation of LoC sensors for agriculture across a wider range of farming practices.

Throughput: LoC systems offer key opportunities in agriculture through miniaturization of analytical processes, enabling on-site testing without trained personnel. They also allow for parallelizing operations, increasing testing efficiency and throughput, making rapid diagnostics and monitoring more accessible for better decision-making and sustainability in agricultural practices.

Concluding remarks

Despite these advancements, challenges persist. LoC technology development needs to focus on improving sensitivity, specificity, and robustness, especially in complex agricultural matrices. Calibration and maintenance of these sensors also remain areas of concern, as they can affect data accuracy over time. Integration into existing farm management systems and the affordability of these technologies for small-scale farmers are other hurdles to overcome.

In conclusion, LoC technology has made significant strides in agriculture by offering efficient, cost-effective, and real-time analysis capabilities. While challenges remain, ongoing research and wider adoption have great potential to further improve the utility of this technology in transforming agriculture towards more sustainable and efficient practices.

Acknowledgments

PhotonHub Europe—One-Stop-Shop Open Access to Photonics Innovation Support for a Digital Europe (Grant Agreement ID: 101016665)

NextGenMicrofluidics—Next generation test bed for upscaling of microfluidic devices based on nano-enabled surfaces and membranes (Grant Agreement ID: 862092)

28. Opportunities for photonic integrated circuits in agriculture and food processing

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Status

Agriculture is one of the biggest industries worldwide with a market size of approximately 12 trillion dollars, accounting for ca 25% of global employment in 2018 [543]. As a result, the demand for resources for agriculture is enormous and is not sustainable in the long term. For instance, agriculture irrigation accounts for 70% of water use worldwide [544] and nitrogen deposition in agricultural areas resulted in a decrease in biodiversity. There is need for more sustainable agricultural production.

'Smart Agriculture' refers to managing farms using modern ITCs to increase the quantity and quality of products while making optimum use of resources and minimizing the environmental impact. It can be regarded as a toolbox of sensing and data technologies including use of sensors, robotics and drones, AI, big data, IoT, and satellites [526]. Photonics based sensing is already widespread in agrifood applications [9]. As technology improves there is a trend towards proximal plant sensing, more autonomous processes, measurement of specific nutrients inside the plant, and further miniaturization of sensing devices.

Process control in the food processing industry is often based on temperature, pH, and pressure as a function of time. Computer vision is commonly used for real-time inspection and grading of fruit, vegetables, and grain ingredients. However, information on the product composition during the process is mainly obtained by time consuming laboratory analyses, and as a result real-time process control based on product composition is not possible. Fast analysis of the ingredient composition is required to replace laboratory analysis. There is a potential for the application of photonic-based spectroscopic sensors that can provide information on product composition to reduce costs related to ingredient storage and real-time process control.

Food producers are legally required to ensure the food safety of their products [545]. In addition, food safety issues can have large impact on a brand's reputations. Food safety includes microbiological, physical, and chemical safety. Physical food safety is related to the presence of foreign matter which represent a hazard upon consumption (e.g. glass, metal, hairs). Microbial food safety relates to presence of the foodborne pathogens that can lead to illness and mortality. Chemical food safety includes e.g. contaminants from the environment and residues of veterinary medicinal products, antibiotics, pesticides, and herbicides.

Agricultural production and food processing require reliable and cost-effective sensors to measure product quality and composition in real-time to replace time-consuming laboratory analysis and to make more optimal use of resources.

Current and future challenges

PICs have great potential in the field of agriculture, as they have the potential to provide small, low-cost, and reliable sensing systems with low power consumption, which fits well with the trends in agriculture (figure 42). Relevant parameters for growth control of crops are growth monitoring, water uptake, transport and transpiration monitoring, and metabolite monitoring, in leaves, stems, and fruit.

In the Netherlands, the government aims to halve nitrogen emissions by 2030 because of the implementation of EU rules to reduce loss of biodiversity. To limit the impact of agrifood production on the environment, it is important to understand the factors that contribute to the decrease of the environmental quality. Fine grained measurement of nitrogen emissions in the environment and in stables requires low-cost, robust, and sensitive gas sensors.

For food processing, promising applications for PIC-based sensors are assessment of ingredient quality, real-time process control, measurement of product properties of the final food product, as well as controlling of food safety along the production process.

However, to develop PIC-based sensors for these different applications, it is necessary to understand the requirements of each application. This includes the specific wavelength ranges, the required frequencies and sensitivities, and application specific requirements, including sample handling and resistance to external factors (temperature, vibration, humidity, etc.). And it is important that specific application requirements are met, but also that the sensors are widely applicable, to maximize market volumes.

For production of PICs-based sensors various building blocks are required. For low-cost spectrophotometric sensors on chip tuneable lasers are needed, with a wavelength tuning range that matches with the application, so that detection can be performed with a photodetector instead of a more costly

Figure 42. On-chip Raman spectroscope developed by imec [545, 546] (top). Silicon photonics wafer technology providing miniaturization and scalability [545, 546] (bottom).

spectrometer [547]. Possible applications are measurement of moisture, lactose, protein, and fat by NIR or MIR spectroscopy [548, 549]. Also, a tuneable single mode laser is suitable to probe the absorption lines of gases in the case of gas sensing. An example is tuneable diode laser absorption spectroscopy (TDLAS) [550]. A wider tuning range makes the sensor more versatile, so that it may be used in other applications. Accurate and highly sensitive detection requires development of photodetectors, detectors for THz, and microphones for photo acoustics applications. For accurate measurements, for instance for gas sensing in the ppb range, longer wavelengths are needed, compare to the traditional wavelengths used for telecom (e.g. C–band = 1530–1565 nm).

Application requirements have a high impact on the optical system design requirements. Analysis of samples that require direct interaction between sample and optical sensor surface, requires physical, mechanical, or chemical cleaning of the optical sensor surface. In case the optical designs become smaller, the possibility to clean these optical windows becomes more limited. Low cost integrated disposable optical sensor heads that can be separated from the optical analysis and electronics may be solution for some cases. For other cases proximal optical sensing may be a better alternative. Other applications require highly integrated and small sensors, e.g. a leaf clip to monitor moisture. However, integrated lasers and light sources are the common denominator for most of the sensing applications.

Advances in science and technology to meet challenges

A limited number of sensing platforms based on PICs, including Vis-NIR spectroscopy, RS, photoacoustic spectroscopy, laser speckle imaging, LiDAR, THz spectroscopy, and biosensing, are suitable to support many of the agrifood applications (table 4). Sensing platforms based on integrated photonics have already been demonstrated, for e.g. RS [546], NIRS [10*], open path gas sensing [547], and photoacoustic spectroscopy [551]. For sensing of emission gasses, specific on-chip lasers are required for each of the relevant gasses, e.g. ammonia and methane, or alternatively tuneable lasers to measure multiple gases using a single sensor. Various materials are available for laser production, each with their own wavelength range, e.g. GaAs, InP, GaN, Si, InAs, and GaSb [552]. Of specific interest is extending the wavelength range of tuneable lasers from the near infrared to the mid infrared region to enable fingerprinting based on vibrations of molecular bonds [553]. Production of tuneable lasers in a cost-effective way requires new production processes, including micro transfer printing [554] and flip chip technology, which are currently being developed.

Accurate and highly sensitive detection requires further development of e.g. resonant cavity enhanced photodetectors [560], waveguide integrated antenna-coupled diodes for THz [561], and low-cost sensitive microphones for photo acoustics applications.

For sensing mostly waveguides in a straight or spiral configuration (longer interaction path with analytes) are used. In the context of RI sensing more complex structures are available (e.g. ring resonators, Mach-Zehnder interferometers, photonic crystals) [562]. For biosensors multiplex capability is relevant

Table 4. Overview of agrifood applications and suitable photonic modules.

Property	Photonic modules
Plants & fruits	
Plant morphology	Lidar [175], 3D Imaging
Plant moisture	THz [555] (100 GHz–2 THz)
Sap flow	Laser Speckle [556]
Plant nutrients	NIRS [548] (800–2400 nm)
Fruit ripeness	NIRS [548] (800–2400 nm)
Pesticides	Raman [557] (SERS; 350–1700 nm)
Storage conditions	Gas sensing [558], laser absorption spectroscopy, photoacoustic spectroscopy
Controlled ripening	Gas sensing [559], laser absorption spectroscopy, photoacoustic spectroscopy
Livestock	
Feed & water quality	NIRS [548] (800–2400 nm)
Emission gases	Gas sensing, laser absorption spectroscopy, photoacoustic spectroscopy [551]
Food processing	
Composition	NIRS [548] (800–2400 nm), MIRS (2400–11 000 nm), Raman (875 nm laser, 300–1800 cm^{-1})
Flavor	Gas sensing [558], laser absorption spectroscopy, photoacoustic spectroscopy
Microbiological safety	Fluorescence, biosensing
Physical food safety	THz imaging [555] (0.1–4.0 THz)
Chemical food safety	NIRS (800–2400 nm), MIRS (2400–11 000 nm), Raman [557] (875 nm laser, 300–1800 cm^{-1})

[563]. To connect various photonic structures in a PIC edge couplers and gratings are required to enable light input/output [564].

To increase specificity, waveguide coatings are essential for the sensor fabrication process. For spectroscopic sensing, metal-organic frameworks or sorbent polymers are available to concentrate target analytes close to the waveguide. For biological and refractive index-based sensing, e.g. antibodies may be attached to waveguides to capture target biomolecules with high specificity [175].

Most examples from scientific literature demonstrate the initial feasibility of PIC based sensors. However, the challenge is to increase the TRL level of the sensors and to develop the manufacturing processes. The photonic sensors market is at a relatively early stage and current manufacturing is focused on telecom wavelengths. Extension of photonic structures to other waveguiding materials to enable sensing at wavelengths beyond the telecom domain is a key goal. Photonic structures of PICs require very high design fidelity, and it is essential to limit manufacturing variability.

Concluding remarks

In conclusion, the markets for sensors are rapidly growing, and Photonics Integrated Circuits (PICs) have great potential in the fields of agriculture and food production, as they have the potential to provide small, low-cost, and reliable sensing systems with low power consumption. Together with availability of low-cost PIC based sensors, the wide availability of cloud computing, and the use of AI to automatically generate models from sensor data, will pave the way to broad application of PICs in the agrifood sector. However, the photonic sensors market is at a relatively early stage, and investments in manufacturing capability are needed to achieve the advances detailed in this chapter. Also, the diversity of agrifood production processes and the big range of sensor devices require a clear prioritization based on economic and societal benefits.

Acknowledgment

This research received funding from the Netherlands National Growth Fund “PhotonDelta”.

Chapter 4: Optimized lighting

29. Wavelength-stabilized and tunable diode laser-based light sources for sensing applications in the agro-food sector

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Status

In addition to customized detection systems, light sources with target-specific requirements are key components in recent optical sensing techniques in agro-food applications. The covered spectral range extends from the UV (100–380 nm) through the visible (VIS: 380–780 nm) and infrared (IR: 780 nm–100 μm), up to the terahertz region (THz: 100 μm–1 mm).

Target spectral regions can vary for different techniques. For example, fluorescence probing electronic transitions requires excitation wavelengths in the UV-VIS. Techniques like lidar and RS based on scattering use light sources from the UV to the near IR range. Absorption spectroscopy where characteristic lines occur in the whole optical spectral range can apply light sources with various excitation wavelengths.

Key specifications of the light sources include emission wavelength, spectral width, spectral tuneability or spectral switching, optical output power, and beam quality. With respect to portable instruments, compact size and low power consumption are additional important factors. Several techniques require continuous wave (cw) operation whereas other applications utilize pulsed excitation.

These requirements can be addressed by compact, reliable, and robust diode laser-based light sources. In various sensor applications, moderate optical output powers up to a few hundreds of milliwatts together with target-specific emission linewidths and spectral tuneability are needed. Here, devices with implemented internal gratings, either realized as distributed feedback (DFB) [559] lasers or as distributed Bragg reflector (DBR) lasers provide the necessary spectral capabilities. The combination of several devices emitting at different wavelengths within one laser chip either as laser bar with several output apertures or combining the light into one common output spot using Y-branch or multi-mode interference (MMI) couplers allows fast wavelength switching. Adjusting the current through DFB lasers or implemented heater elements close to the gratings of DBR lasers enables fast spectral tuning without changing the heat sink temperature. Higher output powers can be achieved by using e.g. flared sections integrated monolithically into tapered lasers (TPL) or as separate tapered amplifiers (TPA) in hybrid master oscillator power amplifiers (MOPAs).

Selected III–V compound semiconductor materials form the basis to manufacture such devices addressing the UV–VIS spectral range (GaN, 3xx-5xx nm), the VIS–NIR spectral range (GaAs, 6xx-11xx nm), or the NIR spectral range (InP, 13xx-20xx nm). Additionally, the application of second harmonic generation (SHG) or sum frequency generation (SFG) can fill gaps in the spectral coverage.

This contribution will focus on internally wavelength-stabilized, spectrally tunable, or spectrally switchable diode lasers for cw or pulsed sensing applications in the VIS and NIR.

Current and future challenges

RS is a well-established analytical tool but suffers from the weakness of the Raman signals in comparison to strong disturbing backgrounds especially in real-world applications (e.g. fluorescence, daylight). A physical approach to address this issue is changing the excitation wavelength by an amount comparable to the spectral width of the Raman signals of the target under study. While the Raman signals follow the change in the excitation wavelength, background signals remain spectrally unchanged, thus enabling an effective separation. In a concept with two wavelengths (SERDS) [565], the Raman signals are obtained simply by subtraction of both measured spectra followed by integration and baseline corrections. Techniques with up to eight different emission wavelengths (e.g. sequentially shifted excitation) [566, 567] require more complex data treatment.

Here, light sources with typical emission widths of about 10 cm^{-1}, output powers in the 100 mW range, and a spectral distance between excitation wavelengths of about 10 cm^{-1} (e.g. 0.6 nm at 785 nm) are requested. One potential but rather slow way is to change the overall device temperature. Shorter switching times can be realized by implementing heater elements close to the wavelength-stabilizing gratings, applying a direct current through the grating section, or the implementation of multi-resonator devices.

In absorption spectroscopy under atmospheric conditions, e.g. using individual rotational-vibrational lines for the determination of gas concentrations, the emission linewidth should be smaller compared to RS. Assuming a full scan of an absorption line, e.g. of water vapor at 940 nm with a linewidth of 0.2 cm^{-1} (20 pm), the emission width should be at least one order of magnitude smaller. Less demanding and fast while still providing sufficient target information would be a dual-wavelength approach and wavelength switching between a wavelength in resonance with the absorption line $\lfloor_{\mathrm{on}}$ and a second off-resonance wavelength $\lfloor_{\mathrm{off}}$. Here, an emission width close to the linewidth would be acceptable.

To illuminate larger areas in RS on targets with heterogeneous material distributions, light sources with Watt-class optical output powers and the discussed spectral properties are required. Even higher output powers at tens of watts in continuous wave or pulsed operation are required to perform gas concentration measurements based on the DIAL. To enhance the optical output power available for applications without sacrificing the spectral characteristics, hybrid MOPA approaches are preferred. The light from an above described wavelength-stabilized diode laser serving as master oscillator master oscillator is focused into a power amplifier. This concept enables to increase the optical output power from the 100 mW range provided by the master oscillator to several 10 W. Moreover, short pulses in the nanosecond or picosecond range can be obtained, e.g. for DIAL.

Advances in science and technology to meet challenges

Externally wavelength-stabilized tunable devices for the above discussed spectral sensor applications are well-established. Also, the concept of MOPAs for the generation of short laser pulses with high peak power, e.g. for lidar applications, is well-known. The realization of such systems in a compact manner requires time-consuming high-precision active alignments and mountings of optical elements during manufacturing. An implementation of gratings as intrinsic wavelength-stabilizing elements during the manufacturing process of semiconductor device reduces the efforts significantly and allows a large volume production.

Several approaches to implement internal grating structures into the semiconductor laser were realized, i.e. writing gratings using holographic exposure, using evanescent metal grating structures, and implementing higher order gratings by using electron beam lithography. Especially the latter technology allows for low-order surface gratings and full wafer processes without any additional overgrowth process.

DBR lasers (figure 43(a)) and DFB lasers (figure 43(b)) were manufactured on a full wafer scale for the spectral range between 635 nm and 1180 nm. At 785 nm, a typical excitation wavelength in RS, a DFB ridge waveguide (RW) laser reached a spectral tuning range of 1 nm suited for the application SERDS [568]. Larger tuning ranges up to 2 nm were realized using a DBR laser with implemented heater elements close to the grating [569]. A further increase of the tuning range could be expected by introducing Y-branch coupled DBR lasers (figure 43(c)) [570–573] or MMI coupled DBR-MOPA devices (figure 43(d)) [574, 575]. The concepts were extended to four (figure 43(e)) [576] or six branches [577] to increase the spectral coverage up to 23 nm at an emission wavelength of 975 nm.

For absorption spectroscopy, DFB lasers are preferred to scan over full absorption lines. In the VIS and NIR, experiments for the determination of oxygen and water vapor concentrations are known. Dual-wavelength diode lasers can be used for the above-mentioned $\lfloor_{\mathrm{on}}$-$\lfloor_{\mathrm{off}}$-approach.

An increase of the optical output power was achieved by coupling the laser emission from the devices from figures 43(a)–(e) into an amplifier figure 43(f) thus realizing cw output powers of 1 W at 785 nm [359]. Pulsing the injection current though the RW gate and the tapered section, pulses suitable for miniaturized DIAL systems with 4 ns length and 15 W output power were reported at 960 nm [578].

Figure 44 presents an overview of achievable cw optical output powers from selected devices. Lasers based on narrow RWs (light blue circles) or dual-wavelength Y-RW or MOPA devices (dark blue circles) reach optical powers up to 1 W. TPAs and lasers (red triangles) enable an extent increase of the output power by at least one order of magnitude.

Concluding remarks

Selected optical sensing techniques in the agro-food sector require target-specific excitation light sources. This contribution presented selected concepts to address these requirements. The above-mentioned monolithic devices are nowadays commercially available or close to the introduction into the market, helping to advance current applications and giving access to entirely new fields of applications. In the future, the biggest issue would be the monolithic integration of MOPA systems. Present physical challenges include the thermal coupling between the different sections and the occurrence of different sub-resonators formed by the facets and the internal gratings. Technologically, the devices will have a larger length leading to a more challenging mounting technology, which should be as much as possible expansion matched to prevent internal strain over the entire resonator length. Also, the reliability of these complex devices could be a potential issue.

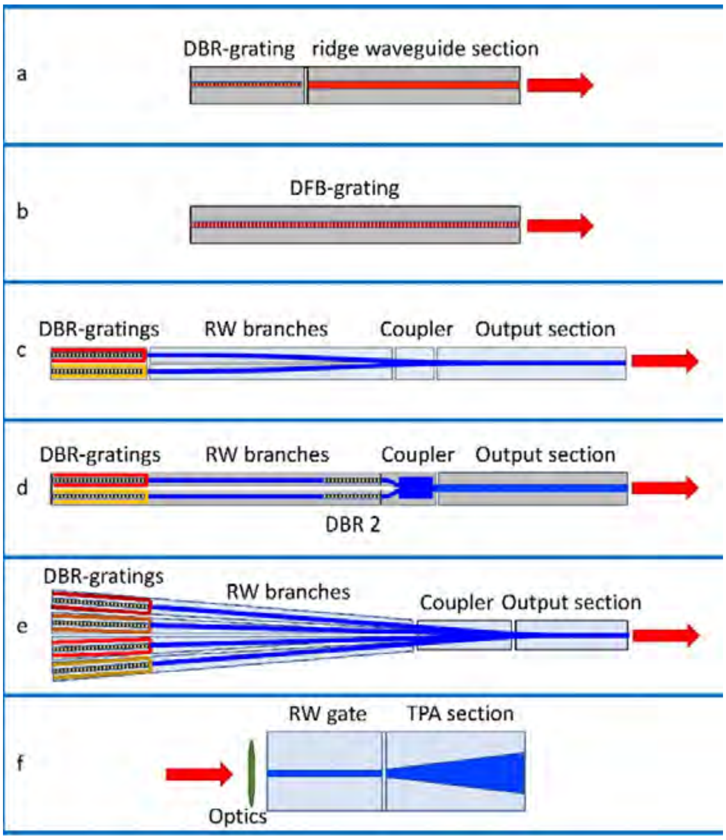

Figure 43. Schemes of selected diode laser concepts with internal wavelength stabilization (a)—DBR-ridge waveguide laser, (b)—DFB laser, (c)—Y-branch DBR RW laser, (d)—MMI DBR RW MOPA, (e)—four-wavelength Y-branch DBR RW laser) and a tapered amplifier (f)—red arrows mark the laser emission in a-e and the input laser beam into the amplifier f.

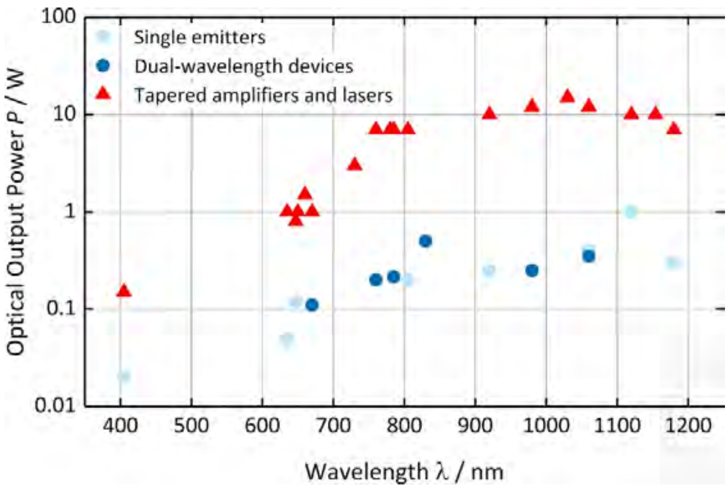

Figure 44. CW output powers from RW DBR and DFB devices (light blue circles: single emitters, dark blue circles: dual-wavelength devices) and RW amplifiers at 405 nm [579] as well as tapered amplifier and lasers (red triangles) [580, 581].

Nevertheless, state of the art manufacturing technology is available, and it should be possible within the next years to implement further features directly into the semiconductor laser and maybe combining the devices into photonics integrated circuits. Here, also the monolithic realization of extremely narrow linewidth devices suitable for quantum technology applications could be on the semiconductor road map.

Acknowledgment

This study received funding from the Federal Ministry of Education and Research (BMBF) within the projects RaMBo (Grant Nos. 031A564C, 031B0513C and 031B1069C) within the funding measure BonaRes (Soil as a Sustainable Resource for the Bioeconomy), DiLaRa (Grant No. 03V0207) and Research Fab Microelectronics Germany—FMD (Grant No. 16FMD02).

30. Advanced mid-infrared light sources for food quality/safety applications

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Status

In recent decades, MIR spectroscopy has evolved into an increasingly relevant analytical technique in food industry for quality control and safety [582]. Conventional MIR spectroscopy applied in this field is based on FTIR spectrometers relying on thermal radiation sources that emit broadband black body radiation usually via resistive heating across a wide spectral window (2.5–25 μm). Typical black body emitters include Nernst glowers and globars [583]. FTIR spectroscopy has gained importance for the analysis of food-borne pathogens like fungal contaminations and intrinsic mycotoxins (e.g. deoxynivalenol (DON), aflatoxin B1 (AFB1), ochratoxin A, etc) in a variety of commodities such as wheat, maize, peanuts, dried fruits [386, 584]. Besides such biopathogens, contaminations resulting from pesticides, herbicides and insecticides have also been investigated [585, 586]. In addition to its role in ensuring food safety, IR spectroscopy is useful for quality control and quality monitoring. This exemplarily includes but is not limited to the analysis of the fatty acid (FA) composition in lipids for characterizing fish and milk quality [587, 588].

Within recent years, advanced narrowband light sources including QCLs—in part combined with external cavities facilitating broad tunability (EC-QCLs)—and interband cascade lasers (ICLs) have become a competitive alternative to traditional broadband light sources also revolutionizing food safety/quality analysis. Lasers provide several advantages compared to broadband emitters including higher output power, operational stability and in part broad tunability (>400 cm^{-1}). Nowadays, tunable MIR lasers are commercially available within the 3–13 μm spectral window, as well as QCLs/ICLs with single emission wavelengths between 2.5 and 14 μm [589]. MIR lasers are particularly suited for chem/bio sensing scenarios when addressing strongly absorbing samples or if high sensitivity is required.

For brevity an exemplary relevant food safety scenarios should be highlighted, i.e. screening of mycotoxins. For that purpose, the detection of DON in maize and wheat below 1250 μg kg^{-1} and the detection of AFB1 in peanuts below 2 μg kg^{-1} has been shown using QCLs operating in the particular spectral range of interest (5.5–6.4 μm) [394]. Moldy peanuts were identified by determining intensity differences of the FA signature around 1710 cm^{-1} [590]. The analysis of proteins (i.e. α-lactalbumin, β-lactoglobulin, bovine serum albumin) serves as a crucial example for quality control in dairy industries, and has been performed via EC-QCLs at concentration levels <0.1 g l^{-1} even in highly absorbing matrices such as water and milk [549, 591]. Hence, utilizing IR laser spectroscopy for screening contaminants provides distinct advantages vs. conventional food analysis methods usually relying on separation techniques—which remain the gold standard for detailed contamination studies—given minimal sample preparation, the potential of direct analysis, the non-destructive nature and reduced cost per analysis. While the current-state-of-the-art in food safety analysis using MIR spectroscopy relies on the application of blackbody emitters, the emerging usage of MIR lasers for target analysis pushes the envelope in terms of sensitivity and addressable matrices.

Current and future challenges

While some challenges associated with the currently applied light source including black body emitters and QCLs remain, alternative technologies such as MEMS and MIR-LEDs are prospective solutions improving the capabilities of MIR chem/bio sensing in food analysis. Figure 45 provides an overview of the currently employed light sources in the context of food analysis and includes emerging technologies expected to be integrated within the coming years along with sample interface strategies and infrared detector technologies.

Nowadays applied MIR light sources in the food safety/quality analysis such as thermal emitters and cascade lasers are still subject to certain limitations and challenges. The light source temperature determines the wavelength range and the intensity of the radiation emanating from thermal emitters. This dependence on temperature limits the utility of thermal emitters in the so-called 'fingerprint region' (6–15 μm) containing relevant molecular information. Furthermore, thermal emitters radiate across a broad wavelength window, which consequently results in reduced energy density per wavelength or narrow wavelength band [583, 589]. Low light intensities together with background noise (e.g. electronic, vibrational or thermal

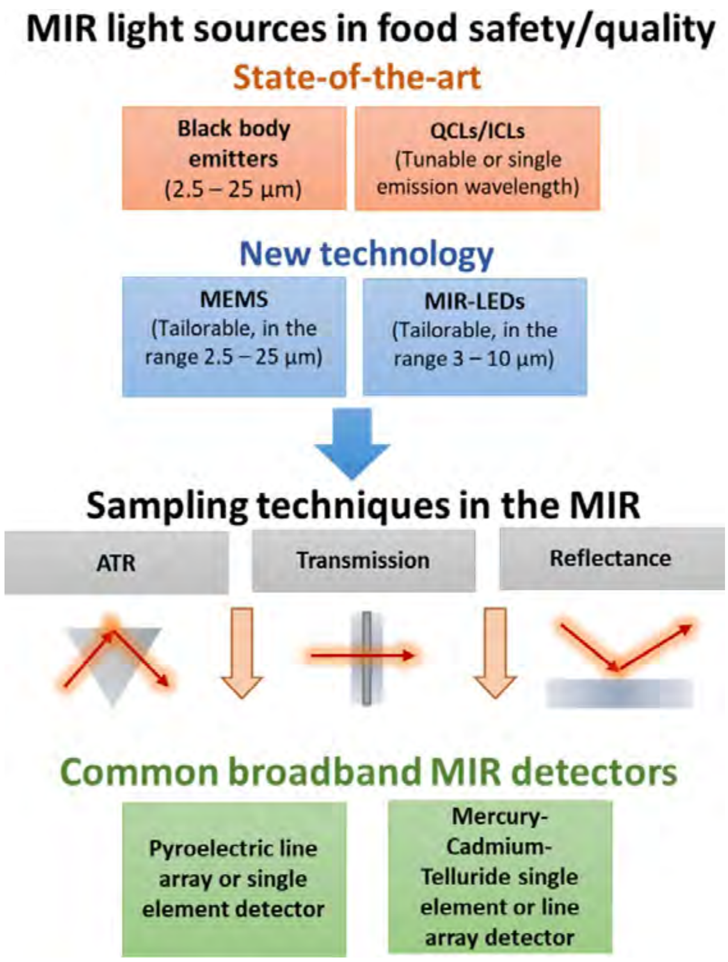

Figure 45. Overview on MIR light sources, emerging technologies, sampling interfaces and MIR detectors relevant in food quality/safety analysis.

noise) affect the overall sensitivity of the device and may restrict applications in food analysis to target analytes present at high concentrations given that the achievable LODs hover around 0.05 g l^{-1} [592].

Despite the evident advantages of using laser light sources, certain limitations remain affecting applications in real-world scenarios in the food industries. ICLs and QCLs are high-intensity light sources that may introduce inherent noise to the system. Hence, real-time referencing is recommended including but not limited to balanced detection schemes [593]. In addition, lasers emit radiation within a limited spectral bandwidth, i.e. even broadly tuneable QCLs do not cover the entire MIR spectral window of interest (2.5–25 μm). Last but not least, lasers typically require complex operation electronics for temperature, current and tuning control rendering ICL-/QCL-based sensing systems expensive, which in turn elevates the entry barrier especially into the food quality/safety screening market demanding for low-cost devices.

When designing portable and compact devices for on-site analysis, both types of MIR light sources usually require light-guiding optics, suitable electronics and appropriate detectors adding to the complexity and dimensions of the sensing system. Last but not least, it should be noted that any MIR sensing system is affected by environmental parameters including humidity and temperature, which may convolute the IR signatures of interest.

Advances in science and technology to meet challenges

Next-generation MIR light sources already in part address some of the previously mentioned challenges and will be pivotal in establishing MIR sensing technologies in food quality/safety application scenarios.

MEMS-based light sources are also thermal emitters, yet, comprising a heating element integrated into a dielectric membrane usually supported by a silicon substrate. In contrast to conventional black body sources, the emitted wavelength range and the intensity of the radiation can be tailored by varying the structure of the MEMS pattern [583]. Exemplarily, applying graphene oxide (GO) coatings at the SiO_2 wafer surface allows increasing the emissivity by up to 150% via coupling of photons with plasmons induced at the GO [594].

Table 5. MIR light sources for food safety/quality analysis.

Light source	Wavelength range	Advantages	Limitations
Black body emitters	2.5–25 μm	Cover the entire MIR range	Limited emissivity in the fingerprint regime
QCLs/ICLs	Tunable up to 300 cm^{-1} in the 3–13 μm regime; Single emission wavelengths available in the entire MIR band	High output power; operational stability; broad tunability	Limited spectral range; introduce noise
MEMS emitters	Depends on the surface structure and can be tailored in the 2.5–25 μm regime	High intensity in the fingerprint range (>5.5 μm); operation at low temperature	When tailored for a specific goal, may be limited for widespread use
MIR-LEDs	Depends on the quantum heterostructure and can be tailored in the 3–10 μm regime	High intensity in the fingerprint range (5.5–10 μm); precise emission wavelength; operation at low temperature	Currently only available in a limited spectral window (<10 μm)

Thus, the intensity limitation of black body emitters at room temperature may be circumvented rendering the fingerprint regime readily accessible.

By combining a MEMS light source with a pyroelectric line array detector (PLAD) paired with a LVF, compact and portable ATR—MIR devices without any moving parts may be established. These devices were successfully tested for the analysis of relevant analytes in food matrices (e.g. mycotoxins, fatty acids, organic solvents) demonstrating the utility of compact MIR diagnostics for the on-site analysis of food constituents. Integrating MEMS sources with ATR-MIR spectrometers offers sensitivities comparable to advanced laboratory FTIR spectrometers while enabling compact handheld devices. For example, FA analysis at 0.0864 g l^{-1} has been achieved using such a device, which is close to the FTIR LOD of 0.0772 g $^{-1}$l [592].

Another type of light source that shows potential in food safety and readily integrates with the PLAD-LVF spectrometer are MIR-LEDs. MIR-LEDs are based on a quantum heterostructure where electrons from the conduction band quantum wells (QWs) recombine with holes in the valence band QWs. Consequently, appropriate alignment of this 'broken' bandgap structure supports emission energies below the bulk bandgap of the two semiconductors by controlling the QW thickness [595, 596]. By appropriately engineering the QW thickness, the central emission wavelength of the MIR-LED can be precisely adjusted. This tunability of the central wavelength allows to target specific spectral regions, therefore increasing the selectivity of the analysis in complex matrices. MIR-LEDs show high emissivity when operated at room temperature leading to enhanced energy efficiency (EUE) and decreased temperature control requirements [597]. In addition, MIR-LEDs readily integrate onto miniature printed circuit boards, thereby facilitating compact portable devices. MIR-LEDs operating in the 3–10 μm spectral window have already been demonstrated [598], which covers characteristic bands of a wide variety of relevant food contaminants and additives.

In summary, the highlighted emerging MIR light sources demonstrate great substantial potential for miniaturized on-site food safety/quality analysis and sensing beyond lasers and conventional thermal emitters. Table 5 summarizes current and emerging MIR light sources in the context of food safety and quality analysis along with the associated benefits and limitations.

Concluding remarks

In this roadmap, recent trends in MIR light source technology for food quality/safety analysis are discussed. Conventional MIR devices that are routinely employed for contaminant analysis and food quality monitoring are predominantly based on conventional black body sources with the emitted radiation modulated via an interferometer. Overcoming the limitations of thermal radiation sources, MIR quantum heterostructure lasers (i.e. QCLs, ICLs) are gaining importance, however, their adoption in food industries remains limited considering the associated high costs.

Emerging alternative light sources are not yet widely utilized in the field of food quality/safety, yet have promising potential especially for low-cost MIR devices and on-site detection of contaminants including but not limited to mycotoxins in cereals and pesticides in crops. MEMS-based emitters provide reduced power consumption vs. conventional black body emitters and facilitate increased emission intensities in the fingerprint regime. MIR-LEDs are probably the most promising future MIR light source enabling precise tailoring of the central emission wavelength, a high degree of miniaturization, operation at room temperature and direct integration into electronic control circuitry. In addition, MIR-LEDs and MEMS sources are significantly less expensive compared to ICLs and QCLs, although this remains a moving target depending on the number of devices produced per wavelength.

In summary, while highly sensitive analysis at ultra-trace levels will probably require laser technologies, rapid on-site screening and monitoring at moderate concentration levels may indeed be realized utilizing MIR-LEDs or MEMS-based light source technology integrated into compact chem/bio sensing devices.

Acknowledgments

This work was supported by the EU Horizon 2020 Project PHOTONFOOD [#101016444] which is part of the PHOTONICS PUBLIC PRIVATE PARTNERSHIP and by the Research Council of Norway via project SFI Digital Food Quality (DIGIFOODS) [#309259].

31. LED light spectrum and its power on the nutrient content in closed plant production CPPS

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Status

Multispectral LED lighting is a vital component in closed plant production systems (CPPSs) as it enables precise regulation of physiological and metabolic processes. This regulation not only enhances nutrient uptake and the synthesis of secondary metabolites such as antioxidants, anthocyanins, and phenolic compounds, but also strengthens the plants' response to stress. The production of these compounds, which are required for stress response, is species and growing condition-dependent. The use of 'light recipes' is a key strategy that allows for the adjustment of growth, water use efficiency (WUE), EUE, CO_2 uptake, biomass accumulation, and final product quality. The qualities (blue, red, green, yellow, infrared, and UV) of light, sensed by specific photoreceptors such as cryptochromes and phytochromes, regulate stomatal opening and root activity, promoting the boost of essential nutrients. These photoreceptors trigger signals that activate the expression of key genes in roots, such as nitrate (NRT1) and phosphate (PHT1) transporters, allowing efficient transport of nutrients into plant tissues. Upon receiving these signals, roots enhance the proliferation of root hairs, thereby optimizing surface area for water and mineral uptake. Figure 46 illustrates the effects of different LED light spectra and light combinations on nutrient and metabolite synthesis in plants. In this context, sustainable lighting strategies are essential to maximize crop productivity and efficiency in controlled systems [599].

Current and future challenges section

Blue light regulates stomatal opening, anthocyanin synthesis, and the expression genes, increasing antioxidants and providing protection against oxidative damage [600]. Additionally, its influence promotes plant morphology and compact growth [601]. **Red light** growths leaf thickness and density and improving leaf structure, its repellent activity on some pests reduces the use of pesticides [602]. **Green light** absorbed in the deeper layers of the plant canopy, regulates metabolic processes, and nitrite content in leaves. Also, it promotes the synthesis of amino acids and essential biomolecules [603]. **Yellow light** is slightly used. However, it reduces the rate of net photosynthesis while increasing the accumulation of carotenoids and flavonoids, which are essential for antioxidant protection and it plays a role in photoperiodic signaling [604, 605]. **UV light** is a factor in the physiological structure of plants. UV-C controlling pathogens, improving the bioactive compounds like glycosylates, and enhancing stress tolerance [606]. UV-A promotes the accumulation of flavonoids and antioxidants, supports photomorphogenesis, and phototropism by enhancing growth [607]. UV-B boosts the production of secondary metabolites as carotenoids, and enhances tolerance to water stress, supporting resistance to pathogens and improving both plant health and postharvest quality [607]. **Infrared** light expands the quality, flavor, aroma, and appearance, increases the sugar content depending on the amount of nitrogen. The addition of infrared light to a spectrum increases biomass and leaf area of plants [608]. LED light recipes in **White + Blue (84:16)** increase the biomass accumulation in different crops, in addition, WB light activate plant physiological activity and the synthesis of compounds such as anthocyanins and ascorbic acid; its application in closed-plant production systems is convenient [609]. The **Red** and **Blue (70:30)** increases the growth and synthesis of compounds (anthocyanins and phenols). It promotes biomass production, improves the concentration of chlorophylls and flavonoids in the leaves, and increases the nutrients route such as nitrogen, phosphorus, potassium, and magnesium [599]. **Red + Blue (90:10)** helps enhanced biosynthesis and chlorophyll accumulation, improving water-use efficiency and promoting biomass accumulation [609]. **Red + Green + Blue (30.6: 44.0: 25.4)** increases biomass in crops such as radish microgreens, lettuce, other green leafy vegetables improve flavonoid and anthocyanin production. The balance of red and blue radiation allows photosynthetic efficiency and antioxidant formation [609]. **Red + Green + Blue (80:10:10)** promotes biomass production, inhibition of potassium accumulation in leaves. In addition, it increases seed yield, accumulation of macro and micronutrients in plants. It contributes to CO2 fixation and increases fresh and dry weight [609].

Advances in science and technology to meet challenges

A concise summary of strategies, methodologies, and technologies developed for the sustainable management of LED lighting in CPPS is presented below (see figure 47).

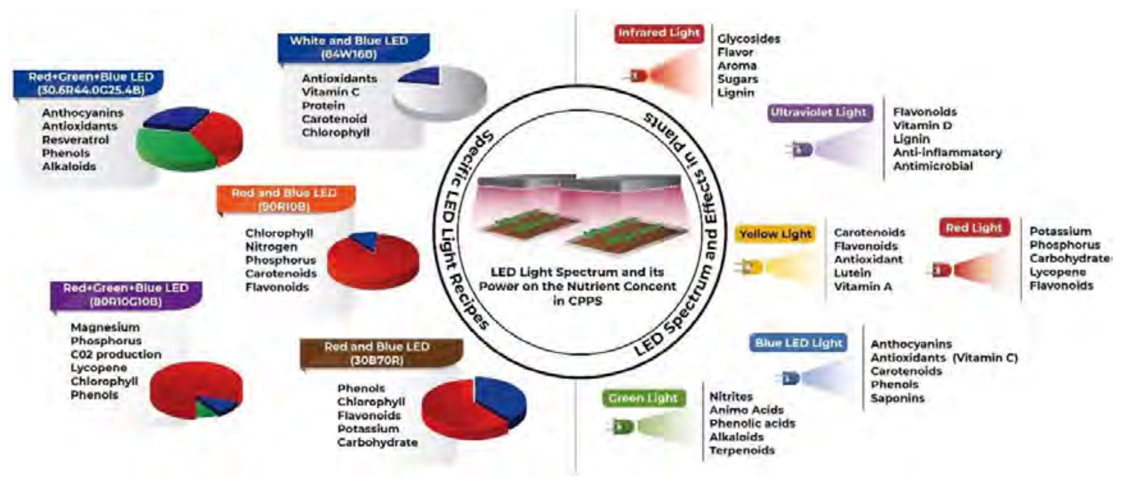

Figure 46. LED light (red, blue, green, infrared) influences the synthesis of specific metabolites and enhancing compounds.

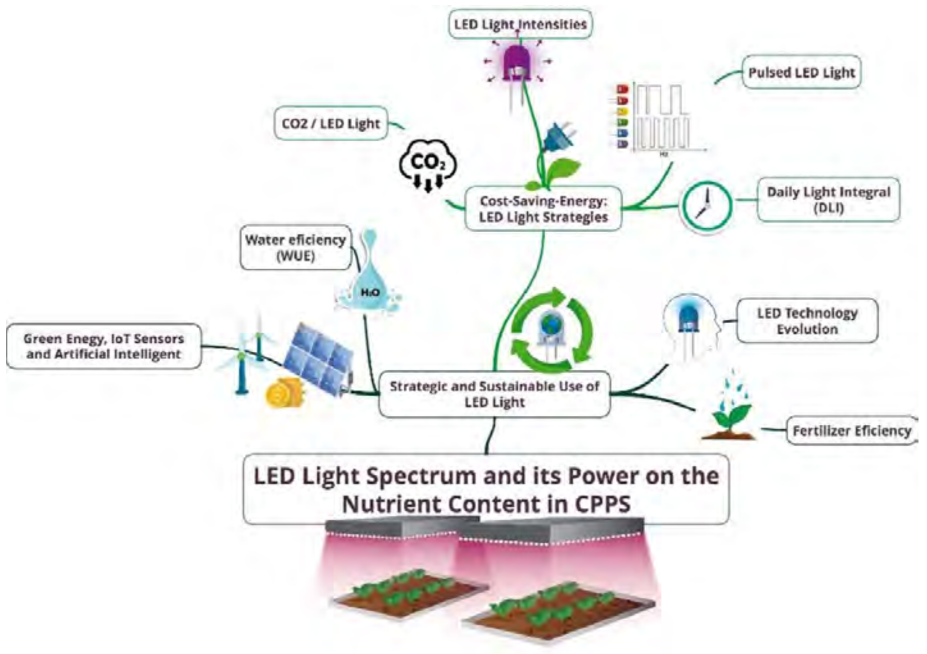

Figure 47. Strategic and sustainable use of LED light in CPPS.

Light/Water/Fertilizers: In CPPS, efficient water use (WUE) is vital, influenced by light factors like intensity, spectral content, and DLI. A balanced mix of these factors enhances WUE [610]. Optimal light intensity is linked to light quality. In addition, excessive light increase transpiration and water usage. Regarding light and fertilizers, the LEDs technology offer diverse spectra, paired with fertilization, to boost nutrient absorption in crops, ensuring human-consumable nutritional levels. Extensive LED spectral research unlocks opportunities to optimize nutrient solutions (micro and macronutrients) for crops in CPPS, yielding innovative strategies for superior growth and quality [611–613]. ***CO2/Light Intensities/DLI:*** Research highlights strong links between CO2, DLI, photoperiod, and light intensities, achieving ideal outcomes in biomass, photosynthesis, weight, nutrient content, and resource efficiency (RUE). Regarding the efficient use of LED light, non-stress threshold light levels and optimal CO2 levels are the key, high light intensities—generating greater energy consumption—do not necessarily yield the best results [614–616]. ***LED technology evolution:*** In considering LED technology for horticulture, two crucial factors emerge: LED costs, linked to reduced investment in CPPS, and photosynthetic photon efficiency (PPE), linked to energy savings. LED manufacturing costs dropped by around 75% from 2014 to 2019, while PPE in white LEDs rose from under 1 μmol/j in 2005 to over 2.5 μmol/j in 2021, with an expected 3.1 μmol/j by 2050. In CM-LED with a red-blue ratio of 4, PPE increased from slightly over 1 ⌠mol/j in 2005 to over 3.1 ⌠mol/j in 2021, projecting over 4.5 ⌠mol/j by 2050 [617]. ***Pulsed LED Light:*** LEDs enable pulsed light control without affecting morphological parameters (dry biomass, leaf area, leaf count, or water usage). However, pulsed light impacts phenolic compounds and antioxidant levels, modifying the nutraceutical value of lettuce. Pulsing also reduces LED energy consumption by 8% to 12%, depending on the light recipe, frequency, intensity, and duty cycle [618, 619]. ***Green technologies, IoT sensors and AI:*** Green technologies like solar panels, wind turbines, storage batteries significantly lower energy cost [618]. IoT and AI will form a powerful combination in vertical farming. For example, IoT sensors can monitor and automate the control of pH, water levels, temperature, and light intensity, as well as manage nutrient solutions remotely. IoT combining with AI can be used for disease detection, highly accurate yield prediction, plant health, leaf and root inspection [620], and also predict LED light energy consumption [621]. AI allows increasing the precision of affordable sensors, reducing the cost of equipment [622]. Implementing IoT sensors in CPPS keeps key growth factors (pH, temperature, dissolved solids, and humidity) within optimal ranges, resulting in significant increases: fresh weight (25%), root weight (36%), dry weight (32%), root dry weight (52%), and leaf count (6%). Nutrients levels, including Ca, Mg, Mn, and Cu, also showed improvement [623].

Concluding remarks

Specific light recipes offer a WUE, EUE, CO_2 uptake, biomass production, and better crop nutritional quality. Blue, red, green, and UV light, are sensed by specific photoreceptors, which initiate a cascade of gene expressions, enhancing nutrient uptake, and antioxidant production. Pulsed LED lighting has demonstrated energy saving benefits while maintaining crop quality. Additionally, integrating green technologies, IoT sensors, and AI in CPPS further enhances precision in controlling growth factors, achieving resource efficiency and promoting sustainability. We underscore the importance of the scientific information available in the literature through two fundamental points:

1. Basic research about the effects of LED technology on plant growth for human consumption remains a topic of great interest to the scientific community. This research continually generates new insights into the phenomena occurring in plant-light interaction.
2. The integration of IoT and AI will be crucial for sustainable crop management in CPPS. Although these technologies may initially increase investment costs due to the level of automation required and higher energy consumption, they offer significant advantages. IoT and AI will be essential in reducing human error, enable continuous monitoring, and supporting the cultivation of higher-value crops in a production system that operates 24/7 throughout the year.

Acknowledgments

We acknowledge the support of the Consejo Nacional de Humanidades Ciencia y Tecnología (CONAHCYT) in Mexico for supporting this work through funds for projects INFRA-2016-01, Project No. 270665. CB-2016-01, Project No. 287818.

32. UV light-based technologies for potential application in the agri-food sector

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Status

UV light is electromagnetic radiation below the visible spectrum with wavelengths ranging from 200 to 400 nm that can be divided into three wavelength ranges: UVC (200–280 nm), UVB (280–315 nm), and UVA (315–400 nm). The UVC region is identified with the highest germicidal effect that corresponds to the peak of absorption of bacterial DNA [624]. The effectiveness of UVC light is derived from its molecular action on DNA, leading to the formation of pyrimidine dimers, primarily thymine dimers. These dimers disrupt the DNA structure, interfering with the processes of replication and transcription, and ultimately leading to the inactivation of microorganisms [625]. Currently, the most common sources of UV light for industrial applications include low- and medium- pressure mercury lamps, excimer lamps, broadband pulsed UV lamps, microwave UV lamps, and LEDs technologies. Each of these has a specific relevance in the agri-food sector for the decontamination of water, surfaces and food [624, 625].

Historical timeline of UV is presented in figure 48. In 1877, Downes and Blunt observed no microbial growth after using sunlight in a bacterial suspension [626]. In 1949, Kelner discovered photoreactivation, which allows bacteria to recover from UV light when exposed to visible light. Eleven years later, Beukers and Berends further elucidated UV light's impact on bacterial DNA by observing the formation of thymine dimers on exposed DNA strands [627]. While the fundamental principles of UV light have remained constant for centuries, the technological advancements and applications of this technology have evolved significantly.

In the early 20th century, Niels Finsen developed the first artificial UV source, employing an electric carbon arc light used to treat lupus vulgaris [627]. Moreover, the production of the first quartz lamp in 1904 by Kuch led to the creation of the first commercial UV mercury lamp for water disinfection in Marseille, France [628]. These early developments laid the groundwork for today's diverse applications of UV light in the agri-food sector, from disinfection to enhancement of food quality. Over time, UV mercury lamps were improved and became the standard for water treatment, waste-water treatment, air purification, and surface disinfection against viruses, bacteria, fungi, and parasites [629]. Beyond disinfection, UV light has found applications in agriculture to enhance plant growth, biomass accumulation, photosynthesis and stem diameter, and increase the resistance to insects and pathogens. This technology also showed to boost nutrient content such as vitamin C, phenols, flavonoids, chlorophyll, carotenoids, and anthocyanins [630]. Vitamin D is an essential micronutrient for the correct functioning of the human body. Apart from sunlight, dietary sources of vitamin D are also important. However, few foods (e.g. mushrooms, blue fish, dairy, etc) naturally contain this vitamin. Notably, the combined effect of UV light with drying processes showed to induce the conversion of ergosterol to vitamin D in mushrooms. The application of UV light for producing vitamin D-enriched mushrooms may be a promising approach for addressing nutritional deficiencies in humans [631].

Despite these remarkable applications, the use of UV light in food industry is still considered an emergent technology by regulatory agencies and the agri-food sector. Further advances in this field could facilitate its implementation in food industry [629]. Furthermore, the emergence of the LEDs technology has revolutionized the UV light source market. The use of UV-LEDs can offer a number of benefits of EUE, operational costs and electricity consumption to the agri-food sector. The higher EUE of UV-LEDs can contribute to a reduction in operational costs and electricity consumption. Additionally, the longer lifetime of UV-LEDs, which also means less frequent replacements, can lead to a reduction in maintenance costs and waste, enhancing the cost-effectiveness of the technology over time. Moreover, the lower heat generation of UV-LEDs is especially beneficial for temperature-sensitive food processing applications, where excess heat could degrade product quality or affect freshness. Furthermore, unlike mercury lamps, their mercury-free design enhances environmental safety, and their adjustable wavelengths and consistent light intensity allow for targeted microbial control without compromising food quality [625, 632]. Ongoing research in UV light promises safer, more efficient, and sustainable solutions for the agri-food sector.

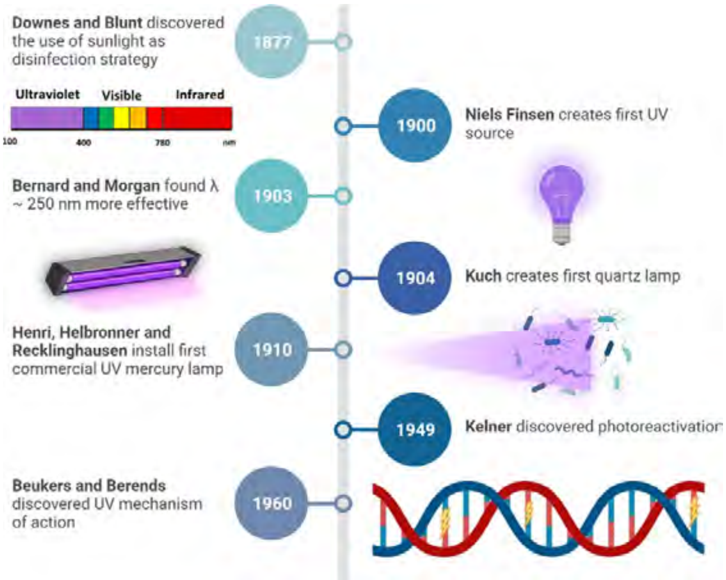

Figure 48. Timeline of UV light discoveries and technological advances (Created with BioRender.com). Information extracted from [625–627].

Current and future challenges

The implementation of UV-based technologies in the agri-food sector requires some challenges to be overcome. Safety and regulatory challenges that consist on ensuring the safety of foods processed with UV light. The regulatory authorities carefully assess and verify the adoption of new technologies. Generally, research must navigate a complex regulatory network to demonstrate the safety and effectiveness of a new technology such as UV light [633]. For instance, the European Food Safety Authority (EFSA) was required to assess the safety of UV light technology for the commercialization of UV-treated bread and cow milk. The novel food EFSA panel evaluated the impact of UV light on the nutritional composition, safety, microbiological quality, and allergenicity of both foods. The panel concluded that the UV light treatment was safe under the intended conditions of use. Other regulatory bodies, such as the Food and Drug Administration (FDA) in the United States, require substantial evidence demonstrating both the safety and efficacy of UV technology for food applications [629]. Addressing these regulatory hurdles is essential for successful adoption in the market.

Apart from safety and regulatory challenges, the agri-food sector must also cope with technical and operational issues in implementing UV technologies. Microorganisms can exhibit high differences in susceptibility to UV treatment. Research is needed to understand the stress response mechanisms of microbial cells involved in UV adaptation and cross-protection mechanisms towards other stresses such as heat, disinfectants, pH, etc [625]. Furthermore, identifying optimal UV doses for different crops and foods is a complex task. UV optimization can be challenging in food due to its low penetrating power. Moreover, the application of UV light to opaque or cloudy liquid foods, powders, or uneven or rough foods can affect the effectiveness of the treatment. The presence of UV absorbing molecules (e.g. sugars, pigments, organic acids, etc.) in foods such as juices may also have an impact on the treatment optimization [634]. Factors such as UV wavelength, intensity, exposure time, and distance from the UV source contribute to achieving the desired results. Researchers need to develop accurate UV dose guidelines for various applications [635]. Currently, standardized guidelines or protocols for UV measurement are lacking. Some studies have proposed the adoption of the nomenclature established by the Photochemistry Commission of the International Union of Pure and Applied Chemistry and recommended the measurement of the photon fluence and photon fluence rate as a means of quantifying the energy applied to water, food or a surface [632, 636].

Consequently, new advances in UV light based-technologies must be taken into account. Although UV-LEDs offer numerous advantages, such as EUE and longer lifespan, their development poses challenges. Researchers should improve the performance, affordability, and availability of UV-LEDs for wider adoption [632]. Thus, although UV technology has proven to be effective in laboratories and small-scale environments, the expansion of commercial agriculture and food processing is challenging. Researchers must design scalable and cost-effective UV systems capable of meeting the volume required by industry. In addition, the introduction of UV technology into existing agri-food processes may be disruptive and expensive. Researchers must develop strategies that seamlessly integrate UV into the current workflow to reduce production delays and costs [637].

UV technology is generally considered to be an environmentally friendly strategy compared to chemical and thermal treatments, but its environmental impact needs to be carefully evaluated. Researchers should conduct life cycle assessments to determine the overall sustainability of UV-based processes [638]. Additionally, long-term research is needed to assess the potential cumulative effects of consumption of UV-treated foods on human health. A primary concern is the potential alteration of nutrients sensitive to UV light, resulting in a change in the nutritional composition of foods. Other concerns include the potential for UV light to induce lipid oxidation, the formation of new photochemical compounds or allergens, the degradation of antioxidants, the generation of off-flavors or the alteration of the food color. The effect of UV light on molecular degradation from a nutritional, quality and sensory perspective has been studied in foods (e.g. vegetables, meat, milk and milk products, etc). Studies evaluating this technology have reported mixed results. The majority of studies have proposed optimizing the UV treatment to maximize the UV effect while minimizing the impact on the nutritional, quality and sensory aspects of food [637]. Finally, consumers' perception of the safety and benefits of UV-treated food is a major challenge. Research into consumer perception and education campaigns is crucial to promote acceptance [639]. Other technologies such as high-pressure pasteurization (HPP) have been gradually adopted in the food and beverage industry. This is a consequence of an increasing consumer concern for minimally-processed, clean label, and organic food products. Strategies for promoting the adoption of technologies among consumers include clear communication and transparency, campaigns focusing on the perceived benefits of their incorporation, and the creation of certifications or labels indicating the safety of the technology [640].

Advances in science and technology to meet challenges

Future efforts should focus on addressing the challenges mentioned above. Improvements in sensor technologies such as UV intensity sensors and pathogenic and spoilage microorganisms' detection sensors could improve the accuracy and effectiveness of the UV treatment. These sensors are designed to detect the presence of an analyte through chemical or biological interactions, providing real-time monitoring and adjustment of food processes such as UV, ensuring consistent results [641]. Moreover, advanced modeling and simulation tools can help predict UV treatment outcomes for specific crops and pathogens. These tools are descriptive and predictive strategies that could help us better understand changes in food microbiology and food quality. Modelling and simulation techniques could facilitate the optimization of UV-based technologies and their system design [642].

UV-LEDs offer many advantages over conventional UV mercury lamps, but they require further development. The advances in UV-LED technology may require to include advances in their design, EUE, and scalability to make them more accessible to the agri-food sector. Innovative design and engineering solutions for UV reactor could address these challenges [632]. Ensuring uniform exposure is crucial for effective microbial inactivation, which can be achieved through rotating systems or multiple UV-LED arrays. Heat dissipation is equally important to prevent damage to food and equipment, requiring the incorporation of cooling systems. Furthermore, UV reactors must integrate seamlessly with existing processing lines, employing modular and compact designs, while maintaining optimized LED placement to ensure EUE. Another critical aspect is scalability, which enables UV reactors to accommodate varying production volumes [629].

Research efforts should focus on establishing industry-wide standards and guidelines for UV treatment protocols, safety standards, and equipment specifications. In the absence of international, clear and standardized guidelines, manufacturers and food processors are confronted with ambiguity regarding the optimal UV treatment, equipment design, and safety assessments necessary for various food types. This lack of clarity impedes regulatory approval and slows market adoption. For example, inconsistent safety protocols across countries presents a challenge to the international trade of UV-treated products [634]. The standardization of UV technology and treatment protocols is essential to ensure consistency and quality in the agri-food sector. To illustrate, the current and widespread use of HPP technology for food application was achieved by establishing clear safety and operational guidelines, thereby ensuring consistent quality and microbial safety [643]. Collaboration between researchers, industry stakeholders, and regulatory bodies can lead to this standardization effort. At the same time, efforts should be made in cooperation between researchers, regulators, and industry players to streamline the approval process for UV-treated foods. Clear guidelines and regulations can provide a framework for implementation [634, 644].

Understanding the genetic and physiological mechanisms that influence microbial susceptibility to UV light could help optimize UV treatment protocols. Advances in microbiology such as the incorporation of next-generation sequencing technologies (e.g. genomics, transcriptomics, proteomics…) might contribute to the understanding of the microbial stress response to UV light and the ability of UV light to induce cross-protection to other stresses [625]. As an example, genetic mutations in the bacterial genome caused by UV light exposure can be identified through the use of Whole Genome Sequencing [645]. Insights such as mapping genetic mutations, studying gene expression changes or understanding protein-level responses may assist in the optimization of UV light inactivation treatment protocols by enabling the tailoring of UV doses to exploit microbial vulnerabilities, thereby reducing the likelihood of resistance. Furthermore, an understanding of how UV exposure induces cross-protection against other stresses (e.g. heat or disinfectants) can inform the development of more effective combination treatments that prevent adaptive microbial survival [625]. Consumer acceptance is one of the most important challenges to be faced by the implementation of UV light on the agri-food sector. Confusion of consumers of UV light with ionizing radiation (or radioactivity) may affect the acceptance of this technology. Advances in communication technologies could promote the education and acceptance to new technologies. Interactive applications, augmented reality, and virtual reality experiences may help consumers understand the benefits and safety of UV-treated food products [646, 647].

Concluding remarks

Past and present advances in UV light technologies have contributed to their increasing interest and promising applications in the agri-food sector. Despite the potential of these technologies, several challenges must be overcome to ensure their successful integration in the agri-food processes. Safety and regulatory concerns require careful navigation, with a focus on microbial response mechanisms and precise UV dose guidelines. UV-LEDs offer several benefits but need further development to improve scalability and affordability. Environmental sustainability and long-term health effects require rigorous assessment, while consumers' perception remains a major challenge. Effective communication and education efforts are essential to promote acceptance among consumers. Moreover, future efforts should prioritize improvements in sensor technology and modeling and simulation tools for the accurate application of UV treatment. This can be also achieved through the use of novel techniques to enhance the understanding of microbial mechanisms towards UV light. Furthermore, other advances in technology such as advances in design and scalability may facilitate the adoption of this technology at industry level. Collaborative efforts from scientists, industry stakeholders, and regulatory bodies are essential to drive the development and implementation of the UV technology in agri-food applications while ensuring safety and compliance with regulations. Future research should prioritize the refinement of UV-LED effectiveness, the optimization of dose guidelines for diverse food types, and the development of robust sensor technology to monitor and control UV exposure with precision. These subsequent steps could facilitate the broader integration of UV technology in agri-food processes over the next decade, potentially leading to its routine use across various stages of food production.

Acknowledgment

This word was supported by the Department of Agriculture, Food, and Marine (DAFM) project CAMPYDECON: Controlling Campylobacter Contamination in Poultry Processing.

33. UVC-LEDs for water treatment

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Status

For more than 100 years, UV radiation has been used in drinking water disinfection, as well as in wastewater treatment, as the process does not require any chemicals and thus does not affect the taste of the water. For this purpose, almost exclusively low-pressure (LP) mercury lamps with a typical emission wavelength of 254 nm are employed and wall-plug efficiencies (WPE) in the range of 20%–40% [648]. In large-scale water treatment plants, medium-pressure lamps (MPLs) are also used since these systems can provide higher irradiation powers. The geometric shape of these radiation sources offers few design options for UV water disinfection reactors. Therefore, disinfection systems are usually cylindrical and the radiation source is surrounded by the water to be disinfected. However, all these lamp types contain mercury, which is harmful to the environment and to human health. Hence, the utilization of mercury is subject to growing regulations in numerous countries, with ongoing initiatives aimed at further limiting its usage, potentially leading to a comprehensive ban. For example, due to the new EU Eco-design Rules for light sources as well as RoHS regulations, a total ban of mercury containing fluorescent lamps was implemented within the European Union in 2023 [649]. However, water disinfection is a mandatory requirement in many regions worldwide because of hygiene concerns, and a ban can only be implemented once a viable alternative technology becomes accessible. Recent advancements in UV LED technology, particularly the improvements in optical power and WPE, have already led to first LED-based disinfection solutions in water treatment. Even though the focus is currently on smaller systems for point-of-use (PoU) and point-of-entry (PoE), there are also first prototype implementations of LED-based systems on an industrial scale. Even though the WPE of UVC-LEDs (UV-C LED) is currently lower compared to conventional mercury discharge lamps the development of UVC-LED-based water disinfection systems has gained significant momentum since these systems offer clear advantages due to their unique properties. For example, UVC-LED based water disinfection system enable a much higher microbiological effectiveness. In contrast to mercury lamps, the emission wavelength of LEDs can be tuned by the manufacturing process to ideally fit the peak efficiency for damaging the DNA of microorganisms (i.e. viruses, bacteria, molds) which is in the wavelength range between 265 nm and 270 nm. Figure 49 shows an example of the microbiological efficacy for some selected microorganisms as well as the emission spectra of a LP mercury lamp (blue) and a 265 nm UVC-LED (red). As can be seen, the spectrum of an UVC-LED is much broader than that of a mercury lamp, but in comparison the 265 nm UVC-LED would be the most efficient radiation source for the inactivation of microbes as it emits close to the peak wavelength of the efficacy curves.

Current and future challenges

Another advantage of UVC-LED based water disinfection systems is clocked operation, since UVC-LEDs provide full irradiation power within fractions of a second after turn-on and they also allow many switching cycles without degradation. These are significant advantages compared to mercury lamps which require several minutes to reach full power and suffer from premature ageing if exposed to frequent switching. As a consequence Hg lamp based disinfection systems usually operate 24/7 even when no water is flowing and thus consume an unnecessarily large amount of electrical energy. In contrast, UVC-LED based systems can be turned on-and-off as needed and their output power can be controlled electronically to match the required irradiation dose levels. Therefore, despite their currently lower WPE and higher purchase price, already today UVC-LED based water treatment systems can be more cost-effective over their service life and are likely to be more efficient due to their higher microbiological effectiveness. An additional hurdle for the practical implementation of UVC-LED water disinfection systems in real-world scenarios are outdated standards and regulations. In many countries, e.g. the US and EU, UV water disinfection systems, especially for municipal use, can only be put into operation after they received successful certification in compliance with local regulations. However, these regulations are generally based on classic mercury-containing radiation sources, which only have a narrow-band emission peak at 254 nm. The benefits, that UVC-LEDs provide, like a broader emission spectrum as well as variable wavelengths and even combinations of

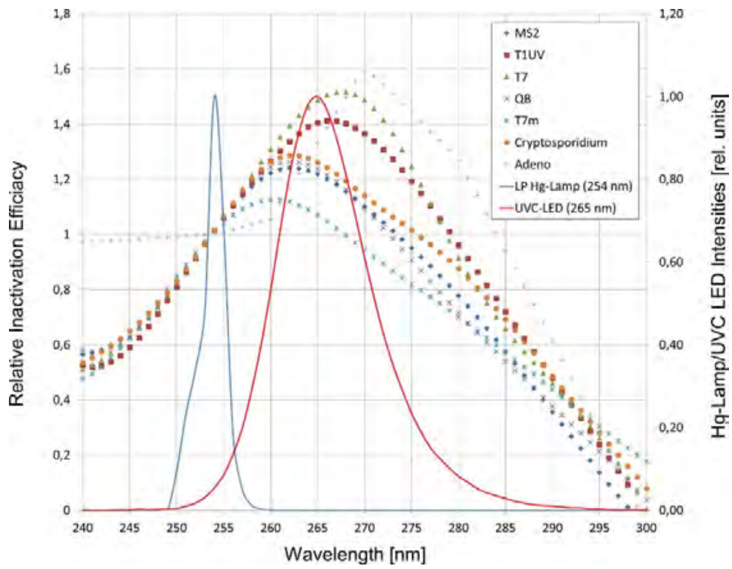

Figure 49. Wavelength dependent microbiological efficacy function for different microorganism (dotted lines, with indicated efficacy on the left *y*-axis) and emission spectra for a low pressure Hg lamp as well as a 265 nm UVC-LED (full lines, with indicated intensities on the right *y*-axis) [650].

wavelengths have not yet been taken into account. Nevertheless, there are currently enormous efforts in regulatory bodies and standardization committees to close these gaps and to create specifications for carrying out the biodosimetric evaluation of UVC-LED-based water disinfection systems. The small form factor of UVC-LEDs and the much greater freedom for the design of UVC-LED radiation sources leads to another regulatory challenge. While almost all Hg lamps have a similar footprint and radiation pattern, even when produced by different manufacturers, UVC-LEDs offer many more possibilities in terms of array design and are UVC-LED modules are currently always customized products. On the one hand, this is advantageous because the radiation source can be optimally adapted to the irradiation problem, but it also leads to the fact that standardization is more difficult. In addition monitoring UVC-LED based systems is more challenging or at least different from mercury lamps which emit almost uniformly over their entire length. For example, in UVC-LED arrays devices can individually fail or age differently leading to a change in the spatial distribution of the radiated power. To remedy the use of multiple UV sensors, their optimal quantity, and their placement within the reactor is currently being investigated. In addition, monitoring of the electrical parameters such as operating voltage or currents might allow failure detection of individual devices.

Advances in science and technology to meet challenges

As can be seen from figure 50 within the past decade the performance characteristic of AlGaN-based UVC-LEDs has significantly improved with WPE in the range from 5%–8% and output power levels exceeding 100 mW for the current generation of commercial devices [651, 652]. These steady improvements have been made possible by gradual advances in group III-nitride materials and device technology, which led to improvements in the radiative recombination efficiency (RRE), the carrier injection efficiency (CIE), the light extraction efficiency (LEE), and operating voltages V [653, 654]. Explaining all the details of the different technological advances would require much more space that this short paragraph provides, but just to list a few. For example, the RRE of UVC light emitter has greatly increased by the development of low defect density templates utilizing high temperature annealing of sputtered AlN base layers on sapphire substrates [655, 656]. In addition, the design and growth of high quality AlGaN materials and QWs by metalorganic vapor phase epitaxy (MOVPE) has considerably progressed, e.g. by reducing the point defect densities, by controlling the optical polarization of light emission as well as by maximizing the radiative recombination rate, thus contributing to the further improvement of RRE. The CIE has also gradually improved by optimizing the electron blocking heterostructure and utilizing polarization doped hole injection layers. Finally, increases in LEE have been achieved via the development of UV-reflective metal contacts as well as utilizing UV-transparent and UV-stable encapsulates [657]. Operating voltages have been reduced and are now typically ranging between 5.5 V and 7 V for commercial grade devices that are driven at dc currents between 250 mA and 500 mA. Taken all together, the currently most advanced commercial UVC-LEDs in the 265 nm wavelength band are reaching WPE and external quantum efficiency (EQE) around 8% and 12%, respectively, which can be attributed to a high internal quantum efficiency (IQE)

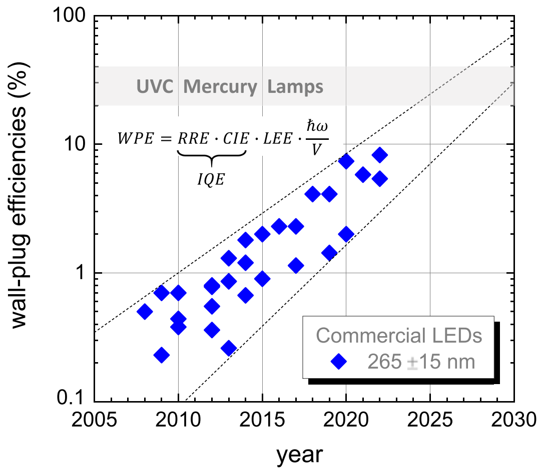

Figure 50. Improvement of wall-plug efficiency WPE (and price-per-Watt) for commercially available UVC-LEDs in the 250 nm—285 nm disinfection band. The dotted lines are a guide to the eye.

$\sim$80%, i.e. the product of the RRE and CIE [658]. Despite all the progress, however, the LEE is still lagging, with maximum values still ranging well below 20%. Therefore, the development of novel approaches to enhance the light extraction will be crucial for future improvements of the WPE and output power of UVC-LEDs. On the upside, the lifetimes of UVC-LEDs have already reached sufficiently high values for real-world-applications with major manufacturers quoting L_{70} numbers of 10.000 h and higher.

Concluding remarks

Despite a number of remaining challenges to the realization of high performance UVC-LEDs, it is clear that the next few years will provide a steady improvement in all UVC-LED WPE, output power, and device lifetimes. These advances are driven by big players, like Nichia and ams-Osram, as well as start-ups entering the UVC-LED market. Extrapolating from the past performance development trends and the aggressive roadmaps provided by device manufacturers one can anticipate that the WPE of UVC-LEDs will reach the 20% mark well before the end of this decade. It is clear that semiconductor-based UVC emitters are poised to further advance in all areas of water disinfection, especially in light of an impending ban for mercury-based UV sources.

Acknowledgment

This work was partially supported by the German Federal Ministry of Education and Research (BMBF) within the 'Advanced UV for Life' consortium.

Concluding remarks

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Photonics is a key enabling technology driving the increased digitalization and smart farming within the agrifood industry. A continued transformation from traditional food systems to Agriculture 5.0 is indispensable to evolve towards a sustainable food and agriculture production. This roadmap aims therefore to provide an overview of the state-of-the-art photonics technologies benefitting agrifood applications.

Optical monitoring and sensing devices, including both imaging and spectrometry systems, have shown promising performances along the full supply chain. In general, advances are observed along different spectral bands from the UV to the terahertz wavelength range, and considering different technologies, including absorption, fluorescence, Raman, and Fourier-transform spectroscopy. A trend towards multimodal sensors is observed, combining different sensing technologies within a single unit or device, offering an improved sensitivity and broader use, while also benefitting the data quality and increasing the sensor robustness. In addition, miniaturization towards handheld devices and PICs is a key innovation field, offering the potential for robust, low cost, low power, easily integrable and operatable sensors. Miniaturization of the optical sensors currently often goes at the expense of the sensitivity and genericity, which can be tackled by combining different precise sensing functionalities.

ML and AI are boosting the processing of optical data. The generation of clear and reliable data is key, while efforts should be made to standardize data enhancing sensor-data fusion. Co-optimization of the sensor hardware and processing algorithms is considered as key to excelling, while care needs to be taken to ensure a successful integration within the application devices (e.g. drones, robots).

The synergy between photonic technologies and data processing presented in this roadmap is a powerful toolset for addressing environmental challenges comprehensively. This integrated approach allows a better conservation of environmental resources as well as mitigation of wastes, thus reducing the environmental impact of food production, and fostering a more sustainable and resilient ecosystem.

New farming strategies, including vertical farming, are becoming a reality, and are benefitting from novel sensing and lighting technologies. Indeed, energy-efficient LEDs and lighting algorithms have indicated to optimize growth and yield, while the combination with spectral imaging systems offers the potential to monitor crop health.

Concluding, this roadmap indicates the revolutionizing capabilities of the photonics technologies inspiring future applications and developments towards a sustainable planet by enabling resource optimization, increased crop yields, stopping land degradation and reduction of food waste.

Data availability statement

The data that support the findings of this study are available upon reasonable request from the authors.

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