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Review

Near- and Mid-Infrared Spectroscopy for the Rapid and Non-Destructive Analysis of Wheat Flour and Wheat-Based Products: A Review

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ABSTRACT

Wheat flour and its derivatives are staple foods worldwide, making their quality and safety essential for the food industry and consumers. Conventional analytical methods are often slow, costly, and destructive. In recent years, infrared spectroscopy, particularly near-infrared (NIR) and mid-infrared (MIR), has emerged as a rapid, cost-effective, and non-destructive alternative for wheat flour assessment. This review summarizes recent advances in applying these techniques to determine quality parameters, monitor functional properties, detect adulterants, verify authenticity, and evaluate contamination risks. The integration of spectroscopy with chemometric methods and machine learning has improved predictive accuracy and robustness, supporting real-time and in situ analysis. In addition, the use of calibration models, wavelength selection strategies, and deep learning approaches has further enhanced analytical performance. Overall, NIR and MIR spectroscopy stand out as key tools to optimize quality control and safety in wheat flour, contributing to fast, reliable, and sustainable analytical systems for the food industry.

Abbreviations: ADA, Azodicarbonamide; ALGL, Albumin/Globulin; ANN, Artificial Neural Network; ATR, Attenuated Total Reflectance; ATR-FTIR, Attenuated Total Reflectance – Fourier Transform Infrared Spectroscopy; BC, Baseline Correction; BPO, Benzoyl Peroxide; CARS-IBPSO, Competitive Adaptive Reweighted Sampling integrated with Improved Binary Particle Swarm Optimization; CNN, convolutional neural networks; COE, Constant Offset Elimination; CP, Crude Protein; DA, Discriminant Analysis; DT, Detrending; ELISA, Enzyme-Linked Immunosorbent Assay; ELM, Extreme Learning Machine; EMSC, Extended Multiplicative Signal Correction; FCM, Fuzzy Cognitive Map; FD, *Fusarium* Damage; FHB, *Fusarium* Head Blight; FT-MIR, Fourier Transform Mid-Infrared Spectroscopy; FT-NIR, Fourier Transform Near-Infrared Spectroscopy; FTIR, Fourier Transform Infrared Spectroscopy; GFS, Gaussian Filter Smoothing; GPR, Gaussian Process Regression; HMW-GS, High-Molecular-Weight Glutenin Subunits; HSI, Hyperspectral Imaging; IDF, Insoluble Dietary Fiber; IPD, Intestinal Protein Digestibility; IRS, Infrared Spectroscopy; iSPA-PLSR, Interval Selection Successive Projections Algorithm + Partial Least Squares Regression; KNN, K-Nearest Neighbors; LASSO, Least Absolute Shrinkage and Selection Operator; LDA, Linear Discriminant Analysis; LMW-GS, Low-Molecular-Weight Glutenin Subunits; LOD, Limit of Detection; LOQ, Limit of Quantification; MA, Moving Average; MC, Mean Centering; MIR, Mid-Infrared Spectroscopy; MN, Mean Normalization; MSC, Multiplicative Scatter Correction; NAS, Net Analyte Signal; NIR, Near-Infrared Spectroscopy; NIR-HSI, Near-Infrared Hyperspectral Imaging; NMR, Nuclear Magnetic Resonance; OSC, Orthogonal Signal Correction; OTA, Ochratoxin A; PCA, Principal Component Analysis; PCR, Principal Component Regression; PGI, Protected Geographical Indication; PLS, Partial Least Squares; PLS-DA, Partial Least Squares Discriminant Analysis; PLSR, Partial Least Squares Regression; RBF-NN, Radial Basis Function Neural Network; RMSEC, Root Mean Square Error of Calibration; RMSECV, Root Mean Square Error of Cross-Validation; RMSEP, Root Mean Square Error of Prediction; RPD, Ratio of Prediction to Deviation; RS, Raman Spectroscopy; SC, Standard Scaling; SCM, Spectral Centering Method; SD, Second Derivative; SDF, Soluble Dietary Fiber; SFS, Spectral Fluorescence Signatures; SGD, Savitzky–Golay Derivative; SGS, Savitzky–Golay Smoothing; SIMCA, Soft Independent Modeling of Class Analogy; SNV, Standard Normal Variate; SOA-SVR, Starfish Optimization Algorithm – Support Vector Regression; SPA-MLR, Successive Projections Algorithm – Multiple Linear Regression; SVM, Support Vector Machine; SWIR, Short-Wave Infrared; TPC, Total Phenolic Content; UV, Ultraviolet; VN, Vector Normalization; Vis-NIR, Visible-Near-Infrared; WT, Wavelet Transform; XRD, X-ray Diffraction; ZEA, Zearalenone.

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1. Introduction

Wheat (*Triticum* spp.) is one of the most cultivated cereals in the world (Çetin-Babaoğlu et al., 2020). Globally, it ranks among the top three most produced agricultural commodities, with an average annual production of approximately 750 million tonnes between 2013 and 2023, surpassed only by sugarcane and maize and comparable to rice (FAO, 2025). Wheat flour is the main ingredient for many food formulations such as bread, cakes, pasta and cookies (Guzmán et al., 2022). As a crucial consumable ingredient, wheat flour offers a rich nutritional profile including carbohydrates, fiber, proteins and minerals (Zareef et al., 2021). Its high production level underscores its vital role in global food security, particularly in temperate regions where its cultivation is concentrated.

Nevertheless, adulteration and subpar quality parameters present challenges to quality and safety assurance, as they can be difficult to detect and pose risks to public health (Zhang et al., 2022). Therefore, ensuring the quality and safety of wheat flour and its derivatives is paramount for the food industry. The development of an analytical method that is rapid, economical, and effective is essential.

The main quality parameters of wheat flour are routinely assessed using standardized AOAC methods (AOAC, 2019). These parameters include key components of the chemical composition, such as moisture, protein, ash, and wet gluten contents (Cornell & Hoveling, 2020). Moreover, technological parameters are evaluated, such as the sedimentation value, falling number and rheological properties as alveograph and farinograph parameters of wheat flour dough. However, the traditional analytical methods used in evaluating the quality of wheat flour and their derivatives are mostly laborious, time-consuming and destructive. Additionally, enzyme linked immunosorbent assay (ELISA), polymerase chain reaction (PCR) and liquid chromatography coupled with mass spectrometry (LC-MS) are also used, but all of these are expensive, need for chemical reagents and require tedious sample preparation (Badaró et al., 2022; T. Czaja et al., 2018).

As a result, non-destructive spectroscopic methods have emerged as a robust alternative. These techniques include hyperspectral and multispectral imaging, nuclear magnetic resonance (NMR), Raman spectroscopy (RS), infrared spectroscopy (IRS), near-infrared spectroscopy (NIR), mid-infrared spectroscopy (MIR), ultraviolet spectroscopy (UV), visible, fluorescence, and X-ray-based methods (Mohd Ali & Hashim, 2022).

Currently, most quantitative spectroscopy has been based on NIR spectroscopy, given its advantages in cost-effectiveness, speed, simplicity, high throughput, portability and versatility (Sadat et al., 2019). On the other hand, the use of MIR spectroscopy is predominantly employed for the qualitative study of molecular structure. This technique allows monitoring fundamental vibrational modes of molecules, which can produce a chemical profile of a specific sample and report on its structure (Du et al., 2022).

The applications of NIR spectroscopy for quality and safety evaluation have been reviewed in food products such as cocoa beans (Teye et al., 2020), edible oil (Li et al., 2020), honey (Biswas & Chaudhari, 2024), spices (Oliveira et al., 2019) and horticultural products (Pandiselvam et al., 2022). Although recent reviews have addressed the use of NIR spectroscopy in wheat-based products (Badaró et al., 2022) and wheat flour (Du et al., 2022; Zhang et al., 2022), these reviews only based on near-infrared spectroscopy. Regarding MIR technology, to the best of our knowledge, no review presenting the existing research and potential applications of MIR technique along with chemometrics to determine the quality and safety of wheat flour and its derivative products. Furthermore, up to now, there are still few studies comparing the performance of both techniques in wheat (H. Shi & Yu, 2017). However, there is an interesting point to cover NIR and MIR techniques coupled with chemometrics to provide comprehensive information to expedite the scientific work related to the analysis of wheat flour and its based products.

In this review, new advances in the evaluation of quality and safety of wheat flour and wheat-based products using non-destructive NIR and MIR technologies are described, including the evaluation of authentication; quality parameters, chemical composition and technological parameters; and other safety analysis.

2. Principle of spectral techniques

2.1. Near-Infrared spectroscopy

NIR spectroscopy is a technique that operates in the range of 780 to 2500 nm of the electromagnetic spectrum, which is located between the visible light spectrum and the MIR spectrum (Pasquini, 2018). NIR spectra contain information about the X–H chemical bonds, like C-H, O-H, and N-H (Manley, 2014). As all molecules containing hydrogen can be detected in a NIR spectrum, a wide range of organic materials can be analyzed using NIR techniques, such as water, lipids, starch or proteins (Futami et al., 2016; H. Wang et al., 2019; Zhang et al., 2022).

NIR spectroscopy is widely used for qualitative and quantitative analysis of food products. This technique is particularly valuable for studying bulk materials with minimal sample preparation (Lohumi et al., 2015).

The entire measurement process of Near-Infrared spectroscopy generally involves the following sequential steps (Fig. 1): (i) Initial spectral data acquisition; (ii) Data preprocessing, where noises and baseline shift from the instrument and background are eliminate; (iii) Calibration model establishment, where a set of reference samples with known analytical concentrations is employed to generate a predictive model; (iv) Model validation, where the accuracy and reliability of the calibration model are assessed and verified; (v) Prediction or characterization, where the validated model is applied to analyze unknown samples, providing quantitative or qualitative information about their composition (Cen & He, 2007).

Initially, NIR spectroscopy instruments relied on dispersive technology, which involved making sequential measurements at each wavelength, requiring the grating to be moved between each measurement. This approach was time-consuming and prone to noise, with the detector being the primary source of noise. To overcome these limitations, Fourier Transform Near-Infrared (FT-NIR) spectroscopy was developed. This technology utilizes a monochromator to separate the frequencies emitted by the NIR source, and a detector simultaneously measures the energy transmitted through the sample at each frequency. The use of an interferometer revolutionized the analysis process by generating a unique signal that contains all the infrared frequencies 'encoded' within it. This innovation significantly reduced the time required to analyze each sample, making FT-NIR spectroscopy a more efficient and accurate method for NIR analysis (Abbas et al., 2020; Ozaki et al., 2021).

Due to the diverse interactions between light and samples, NIR spectroscopy can be employed in various spectral modes, including reflectance (specular and diffuse), transmission, interactance, and transflectance (Badaró et al., 2022; Ozaki et al., 2021), as summarized Fig. 2. Transparent liquids can be analyzed using transmission mode, where the pathlength remains constant. In this case, the absorption is solely dependent on the concentration of the absorbing component (Badaró et al., 2022). However, when dealing with opaque samples, diffuse transmission mode is employed, as some light is scattered. In contrast, solid and granular materials, such as wheat flour and its derivatives, are typically measured using diffuse reflection mode (Scotter, 1990). This method captures both the absorbed and scattered light. The amount of scattering through the sample length is so high that the light that can cross the sample thickness is reflected instead of transmitted (Huang et al., 2008).

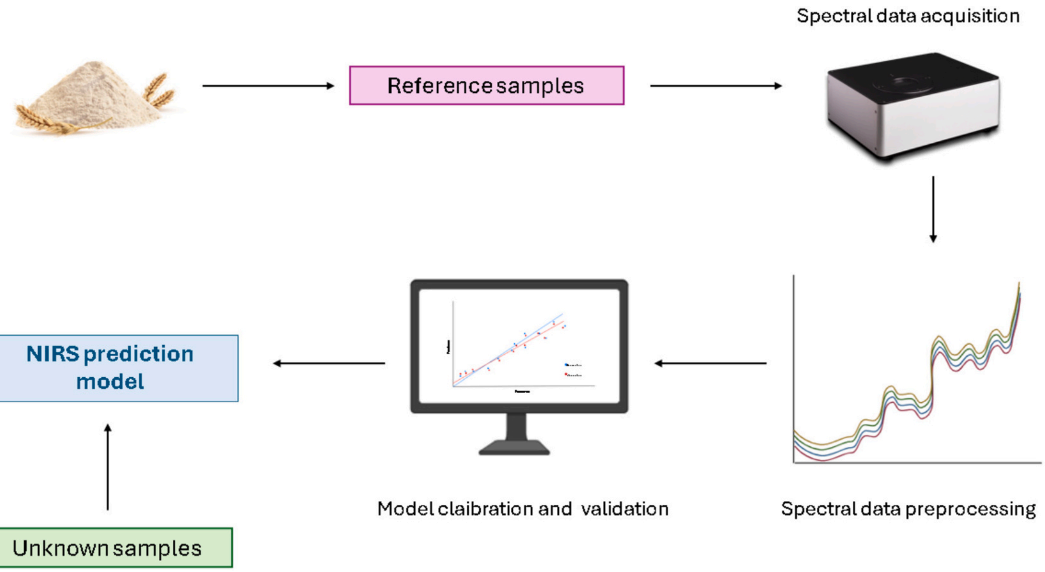

Fig. 1. The main measurement process of Near-Infrared spectroscopy.

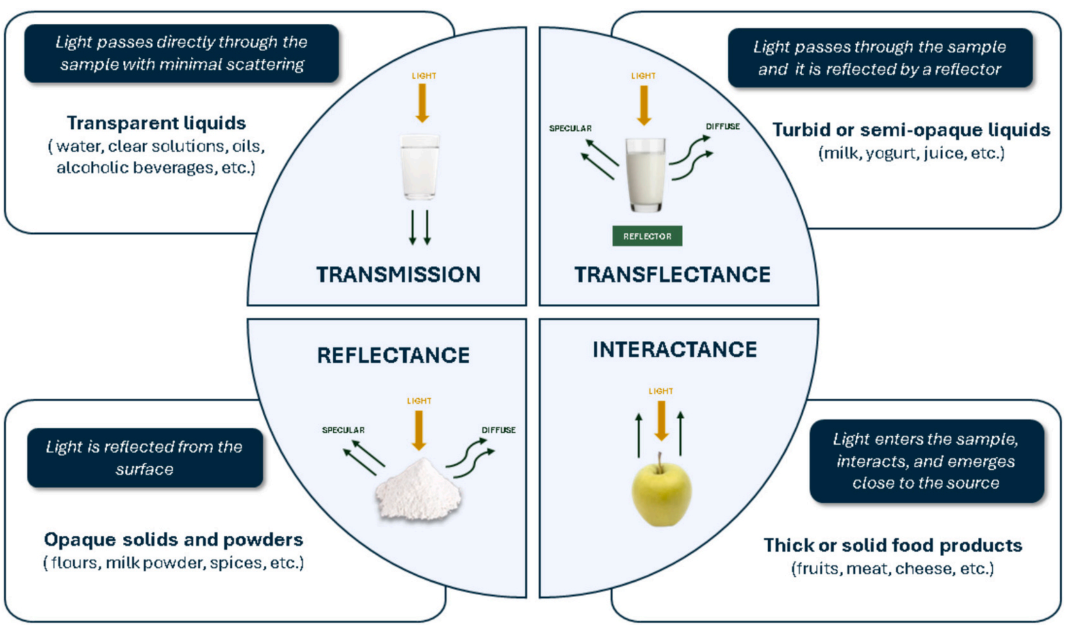

Fig. 2. Light–sample interaction modes applied to spectroscopic evaluation of food systems.

2.2. Mid-infrared spectroscopy

MIR spectroscopy is a powerful technique for structural elucidation and compound identification. Within the MIR radiation range, (4000 to 400 cm^{-1}), specific functional groups absorb photons at characteristic frequencies, providing distinctive spectral fingerprints of the sample. The absorption positions are typically reported as wavenumbers (υ), measured in cm^{-1}. MIR spectra primarily feature bands resulting from fundamental stretching and bending vibrations. Stretching vibrations involve changes in the distance between atoms along the bond axis, while bending vibrations involve changes in the relative positions of atoms perpendicular to the bond axis (Abbas et al., 2020; Colthup et al., 1990). These characteristic spectral features, which reflect the fundamental vibrational modes of specific functional groups, enable the development of analytical methods applicable to a wide range of sample matrices (Carbas et al., 2020).

FTIR has been applied to various food matrices. Recently, FTIR has been increasingly developed for an increasing number of matrices using multivariate analysis approaches. These approaches allow correlation of spectra with chemical data, allowing recovery of analytical calibrations. Furthermore, this technology can be used using different techniques, taking advantage of two spectral regions: the near-infrared and mid-infrared ranges (Carbas et al., 2020; García-Gutiérrez et al., 2021; Hussain et al., 2019).

The main advantages of Fourier-transform instruments include increased sensitivity, much higher energy throughput, superior wavelength resolution, wavelength accuracy and significantly faster spectral acquisition. However, food products present challenges in the Mid-IR region due to their general opacity, high scattering, and significant water content. The development of sample presentation options such as diffuse reflectance (DRIFT), photoacoustic (PAS), and attenuated total reflection (ATR) has significantly facilitated the analysis of such materials. (Downey, 1998; Wilson, 1990; Wilson & Tapp, 1999).

Attenuated total reflectance is a widely used option sampling technique because it requires minimal sample preparation, eliminates variation in cell path lengths and provides consistent spectrum collection. ATR is particularly effective for obtaining spectra of solid samples that are too thick for traditional transmission measurements. The technique operates on the principle of infrared light attenuation when it encounters the interface between an internal reflection element (crystal) with high refractive index properties (e.g ZnSe) and a lower refractive index material (food sample) on its surface (Rodriguez-Saona et al., 2017).

2.3. Near- and Mid-Infrared Spectroscopy: Advantages and Limitations

Although both NIR and MIR spectroscopy are based on molecular vibrational absorption, they differ substantially in terms of spectral origin, analytical selectivity, and practical applicability. These differences strongly influence their suitability for the analysis of wheat flour and wheat-based products.

In general, NIR spectroscopy offers greater robustness for the analysis of heterogeneous wheat matrices and bulk samples, owing to its higher penetration depth, lower sensitivity to water, and compatibility with rapid, non-destructive measurements (Abbas et al., 2020; Reich, 2016). These characteristics make NIR particularly suitable for routine quality control, high-throughput screening, and industrial monitoring across a wide range of wheat-based products.

By contrast, MIR spectroscopy provides higher chemical specificity and enhanced sensitivity to molecular structure, which can be advantageous for applications requiring detailed compositional or structural information (Reich, 2016). However, its more limited penetration depth and higher sensitivity to moisture constrain its applicability in bulk or in-line measurements, particularly for complex or hydrated matrices (Haas & Mizaikoff, 2016; Reich, 2016).

From a methodological perspective, the indirect nature of NIR spectral information generally requires robust multivariate calibration strategies, whereas MIR spectroscopy may allow more direct associations between spectral features and chemical constituents. As a result, NIR and MIR spectroscopy should be viewed as complementary rather than competing techniques, with their relative advantages depending on the analytical objective, sample matrix, and operational context.

A concise comparison of the main analytical and practical differences between NIR and MIR spectroscopy in the context of wheat analysis is provided in Table 1.

3. Chemometrics

Chemometrics is a branch of chemistry that uses mathematical, statistical, and formal logic methods to design and select optimal measurement procedures and experiments. (Héberger, 2008). Chemometric analysis and modeling necessitate high-quality data that accurately reflect the intended measurements (Esbensen & Julius, 2020). This technique allows extracting relevant information from any type of data, including the chemical information from spectra, and correlating it with quality parameters or physical properties of a sample (Caporaso et al., 2017). The application of chemometrics in spectral analysis includes three fundamental steps (Fig. 3): (i) spectral data processing; (ii) calibration model establishment for qualitative and quantitative analysis; and (iii) model transfer (Cen & He, 2007).

Preprocessing the original spectral data is essential to eliminate background information and noise, thereby enhancing the modeling effect. To achieve reliable, accurate, and stable calibration models, it is crucial to preprocess the spectral data before modeling. Numerous preprocessing methods are currently available, including data enhancement, smoothing, derivative, standard normal variate transformation (SNV), multiplicative scatter correction (MSC), and Fourier transform (FT). Additionally, newer methods such as wavelet transforms (WT), orthogonal signal correction (OSC), and net analyte signal (NAS) are also employed (Candolfi et al., 1999; Helland et al., 1995).

Constructing a reliable calibration model for quantitative or qualitative analysis is crucial in food analysis. Recently, many chemometric calibration models have been developed for this purpose. Various approaches are employed in evaluating food quality. Stepwise multiple linear regression (SMLR), principal component regression (PCR), partial least squares (PLSR) are the main methods of quantitative analysis reported in the literature (Cen & He, 2007; Workman et al., 1996). The performance of these models is evaluated using several key parameters: the coefficient of determination of prediction (R^2_P), the root mean square error of prediction (RMSEP), and the ratio of prediction to deviation (RPD). Additionally, the coefficient of determination of calibration (R^2_C) and cross-validation (R^2_{CV}), as well as the root mean square error of calibration (RMSEC) and cross-validation (RMSECV), are also considered. However, it is essential to validate the prediction with independent external data that are not included in the models (Minas et al., 2021; Workman et al., 1996).

Qualitative analysis is also a critical aspect of chemometric methods, involving techniques used to classify samples into specific categories based on prior knowledge. Numerous pattern recognition methods are employed for this purpose, such as linear discriminant analysis (LDA), principal component analysis (PCA), k-nearest neighbors (KNN), cluster analysis (CA), discriminant partial least squares (DPLS), soft independent modeling of class analogy (SIMCA), artificial neural networks (ANN), and support vector machines (SVM)(Ballabio & Todeschini, 2009; Granato et al., 2018; Kamal & Karoui, 2015).

Table 1
Comparative overview of NIR and MIR spectroscopy for wheat flour and wheat-based products.

Aspect	NIR	MIR
Spectral information	Overtones and combinations bands	Fundamental vibrations
Chemical specificity	Moderate	High
Sensitivity to water	Low–moderate	High
Penetration depth	High	Low
Sample preparation	Minimal or none	Surface-limited, minimal (ATR)
Sample size	Large	Low thickness
Suitable matrices	Heterogeneous products	Homogeneous products
Throughput	Very high	Moderate
Portability	Available	Limited
Industrial readiness	High	Moderate
Instrument cost	Moderate	Higher

4. Applications of spectral methods

4.1. Authentication

In recent years, determining the authenticity of food products has become a significant concern for consumers and food authorities (Wadood et al., 2020). Practices such as adulteration, falsification, substitution, and deliberate mislabeling compromise food quality and safety (H.-Y. Liu et al., 2023; Oliveira et al., 2019). Ensuring compliance with appropriate labeling and regulations is essential (Abbas et al., 2018). In this context, the development of rapid, robust authentication methods is crucial, with spectral techniques emerging as an effective and versatile solution (Table 2).

A recent study has evaluated the feasibility of FTIR spectroscopy and multivariate data analysis methods for detecting the adulteration of wheat flour with barley flour (Arslan et al., 2020). The developed SIMCA model demonstrated excellent classification of pure wheat flour, with a detection limit for barley flour below 1%. Additionally, 98.25% of the flour samples were correctly classified using LDA. PLSR models were

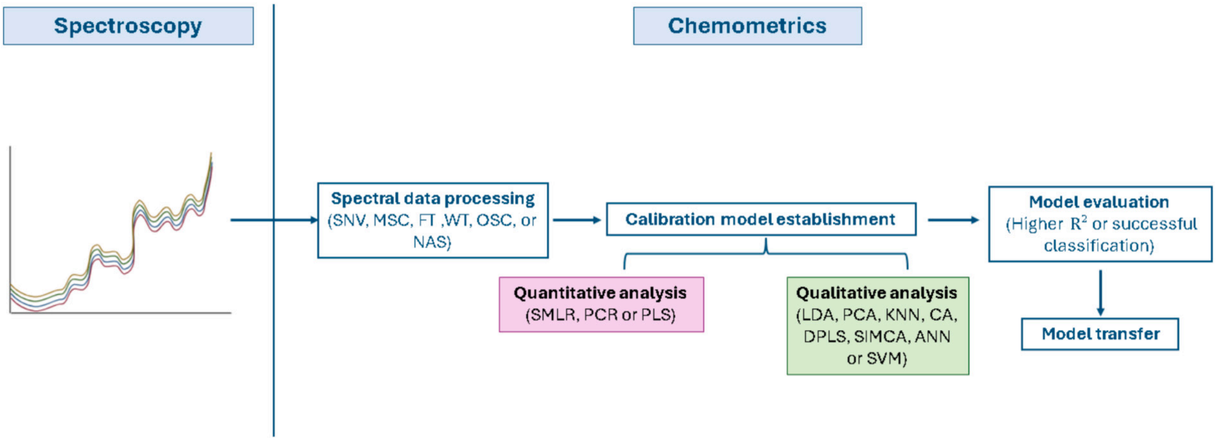

Fig. 3. Scheme of a chemometric method development to evaluate quantitative or qualitative parameters using spectroscopic data.

employed to quantify the level of adulteration. The best predictive capabilities for PLSR were obtained with RMSEC = 0.34–1.34% and RMSECV = 0.36–1.50%. Consequently, barley flour, as an adulterant, could be quantified at levels <0.30% in an unknown wheat flour sample.

On the other hand, pasta holds significant importance in the global market. In some countries, adding common wheat (*Triticum aestivum*) to pasta is considered adulteration, due to the relatively higher price of good quality durum wheat (*Triticum durum*) compared to common wheat (Kamil et al., 2011). Because of this, several studies have investigated the use of non-destructive technologies to detect the addition of common wheat flour to durum wheat flours and pastas. For this objective, different spectroscopic methods were studied by Unuvar et al. (2021) for the discrimination of durum and common wheat samples as a rapid, reliable, easy-to-use, and low-cost tool. A total of 120 common wheat samples and 119 durum wheat samples were analyzed using RS, NIR, spectral fluorescence signatures (SFS) and ATR-FTIR. Data analysis was performed using PCA and Partial-Least Squares Discriminant Analysis (PLS-DA). These spectroscopic tools, combined with chemometric analysis, generally succeeded in distinguishing between common and durum wheat flour samples. ATR-FTIR, and NIR spectroscopy achieved a discrimination rate close to 100% based on high sensitivity and specificity values. In contrast, Raman spectroscopy proved to be the least sensitive method for discriminating between common and durum wheat flour samples, with a relatively high RMSEP value (0.441). Currently, Unuvar et al. (2023) also investigated the use of ATR-FTIR, NIR, and SFS to predict the level of adulteration in durum wheat flours and durum wheat pastas with the addition of common wheat flour. The results indicated that ATR-FTIR had the lowest limit of detection (LOD; 0.68% for flour and 0.49% for pasta) and limit of quantification (LOQ; 2.06% for flour and 1.50% for pasta), making it the method with the highest specificity and accuracy. Similarly, NIR also showed a high predictive performance (LOD of 0.78% and LOQ of 2.38% for flour; LOD of 1.08% and LOQ of 3.27% for pasta) and, due to its widespread use in the food industry, could play an important role in detecting adulteration in durum wheat flour and pasta. However, SFS exhibited a lower predictive capacity for detecting low levels of adulteration (LOD of 5.41% and LOQ of 16.39% for flour; LOD of 2.63% and LOQ of 7.97% for pasta).De Girolamo et al. (2020a) also compared the use of FT-NIR and FT-MIR spectroscopy, in combination with PLS-DA and LDA, to discriminate commercial durum wheat pasta from Italy and Argentina to detect adulteration with common wheat. The results demonstrate that both classification models constructed successfully discriminate against the adulteration of durum wheat pasta with common wheat, with FT-NIR performing better in identifying low levels of adulteration (≤1%), while FT-MIR provided comparable results when a 2% cut-off was applied. Ultimately, FT-NIR and FT-MIR spectroscopy, in combination with chemometric models, present great potential for the promising, rapid and economical detection of the adulteration (Amirvaresi et al., 2021).

The incorporation of ingredients in the formulation of food products can affect their functional, technological, and sensory properties (Wiley & Yen Nee, 2020). The use of rapid and non-destructive techniques to evaluate food quality, specifically wheat flour and its derivatives, has been reported in the literature. Badaró et al. (2019) compared the use of NIR and near infrared-hyperspectral imaging (NIR-HSI) to analyze the quantity, classification, and distribution of added fiber in wheat semolina. Despite the portable NIR spectrometer not achieving satisfactory results in classifying samples with different fiber percentages, NIR-HSI demonstrated sensitivity and specificity values close to or equal to one. Additionally, PLSR models applied to NIR-HSI spectra achieved R_P^2 values ranging exceeding 0.85 and RMSEP values between 0.5% and 1%. The technique proved capable of reliably quantifying fiber additions as low as 2% (the lowest level tested), up to 8%, and provided spatial distribution maps of fiber within the heterogeneous semolina matrix, outperforming the conventional NIR approach. Related to this, Duarte et al. (2022) have investigated the determination and quantification of cassava starch content in wheat flour using NIR spectroscopy and digital imaging. The results of partial least squares prediction exhibited high accuracy with a correlation coefficient of 0.977 and an RMSEP of 1.826 mg·kg^{-1} for certified additive-free wheat flour and a R_P^2 of 0.995 and RMSEP of 1.004 mg·kg^{-1} were observed for commercially processed wheat flour containing chemical additives. These commercial flours contained monocalcium phosphate, sodium bicarbonate, and sodium acid pyrophosphate. The study evaluated cassava starch additions ranging from 3–30% in certified wheat flour and from 1–30% in commercial wheat flour, demonstrating a practical quantification capability down to approximately 1 mg·kg^{-1}. Therefore, this method could be employed to correctly identify samples and prevent food fraud. Similarly, in a recent work, Candeias et al. (2025) also developed an efficient method based on NIR spectroscopy, along with the successive projections algorithm for interval selection in partial least squares regression (iSPA-PLSR), achieving an overall accuracy of 94% to detect and quantify cassava starch in commercial wheat flour, aiming to support the Brazilian bill proposal advocating for the creation of the "Brazilian bread". The study evaluated starch additions from 3 to 30 mg·kg^{-1}, with the best iSPA-PLSR model reaching an RMSEP of 1.376 mg·kg^{-1} and r_{pred} of 0.986, thus demonstrating sensitivity to levels below the lowest concentration tested (3 mg·kg^{-1}).

Furthermore, some chemical additives are often incorporated into wheat flour to standardize its quality and technological properties. Powdered talc and benzoyl peroxide (BPO) are two of the most common additives, chosen for their white appearance and ability to enhance the brightness of the flour. However, their consumption can have adverse effects on human health, making their detection important to ensure

Table 2
An overview of infrared techniques application in authenticity determination of wheat flour and wheat-based products.

Category	Sample	N	Technique	Spectral Range	Objective	Chemometrics			Reference
						Pretreatment	Model	Performance	
Adulteration	Wheat Flour	140	FTIR	4000-450 cm^{-1}	Detection of wheat flour adulteration with barley flour	SNV, SGD	SIMCA, LDA, PLSR	SIMCA: LOD<1% PLSR: R^2> 0.99; RMSEC= 0.34-1.34%; RMSECV= 0.36-1.50% LDA: 98.25% correctly classified	(Arslan et al., 2020)
	Wheat Flour	239	NIR, FTIR	NIR: 900- 1700 nm FTIR: 4000-400 cm^{-1}	Discrimination between common and durum wheat flours	Smoothing, MC, baseline, derivate, detent, normalize, GLSW	PCA, PLS-DA	**NIR** RMSEC=0.158; RMSECV=0,175; RMSEP=0,174 **FTIR** RMSEC=0.186; RMSECV=0,190; RMSEP=0,146	(Unuvar et al., 2021)
	Durum Wheat Flour, Pasta	28	NIR, FTIR	NIR: 900- 1650 nm FTIR: 4000-400 cm^{-1}	Detection of durum wheat flour and pasta adulteration with common wheat flour	Different pre-processing methodologies	PLSR	*Durum wheat flour* **NIR** R^2=0.867;RMSEC=6.642; RMSECV=7.069; RMSEP=9.940 **FTIR** R^2=0.900;RMSEC=6.883; RMSECV=8.602; RMSEP=8980 *Pasta* **NIR** R^2=0.895;RMSEC=9.595; RMSECV=12.926; RMSEP=8.747 **FTIR** R^2=0.903;RMSEC=7.781; RMSECV=9.417; RMSEP=8.908	(Unuvar et al., 2023)
	Durum Wheat Pasta	280	FT-NIR, FT-MIR	FT- NIR: 10,000-4000 cm^{-1} FT-MIR: 4000-400 cm^{-1}	Detection of durum wheat pasta adulteration with common wheat	FT-NIR: BC + DT FT- MIR: MSC + DT	PLS-DA, LDA	**FT-NIR** Accuracy: 85-95% (three classes); 92-97% (two-classes) **FT-MIR** Accuracy: 80-90% (three-classes); 91-97% (two classes)	(De Girolamo, Arroyo, et al., 2020)
Ingredient incorporation	Semolina	140	NIR, NIR-HSI	NIR: 900-1700 NIR-HSI: 928–2524 nm	Identification of fiber addition to semolina	Mean centering, SGD, SNV	PCA, SIMCA, PLSR	SIMCA: Sensitivity: 0.6–1.0; Specificity: 0.9–1.0 PLSR: R_P^2= 0.85–0.98; RMSECV and RMSEP=0.5–1.0 %	(Badaró et al., 2019)
	Wheat Flour	200 (additive-free), 140 (commercial)	Vis-NIR	1100–2500 nm	Quantification of cassava starch in wheat flour	BC, SNV, MSC, SGD	PCA, SIMCA, PLSR	*Additive-free flour* SIMCA: Sensitivity: 100%; Specificity: 94-100% PLSR: R_P^2 =0.977; RMSEP= 1.826 mg/kg *Commercial flour with additives* SIMCA: Sensitivity: 95.5%; Specificity: 100% PLSR: R_P^2 =0.995; RMSEP= 1.004 mg/kg	(Duarte et al., 2022)
	Wheat Flour	125	NIR	900-1700 nm	Quantification of cassava starch in wheat flour	OFF, BC, MSC, SNV, SGD	PCA, PLSR, SPA-MLR, iSPA-PLSR	R_P^2 = 0.995; RMSEP of 1.004 mg kg^{-1}; RPD= 9.682	(Candeias et al., 2025)
	Wheat Flour	41	NIR	400-2500 nm	Prediction of talc content in wheat flour	Smoothing, MSC, SGD, SNV	RBF-NN	Accuracy: 94% R_P^2=0.9999; RMSEP=0.0765; RPD=65.0909	(Liu et al., 2019)
	Wheat Flour	93	NIR-HSI	900-1700 nm	Prediction of talcum powder and BPO in wheat flour	MC, SGD	SCM	Successful discrimination of low levels (<5.0%)	(Fu et al., 2020)

(*continued on next page*)

Table 2 (*continued*)

Category	Sample	N	Technique	Spectral Range	Objective	Chemometrics			Reference
						Pretreatment	Model	Performance	
	Wheat Flour	75	NIR-HIS	900-1700 nm	Prediction of talc and BPO in wheat flour	MC, SGD	Two-Band Spectral Analysis Method	Successfully detected under varying depths of wheat flour	(Fu et al., 2021)
	Wheat Flour	162	NIR	680-2600 nm	Quantification of talc and BPO content in wheat flour	SNV, MSC, SGD, DT	PLSR	R_P^2= 0.995 (talc); 0.964 (BPO)	(Shi et al., 2023)
	Wheat Flour	360	NIR	11,542–3946 cm^{-1}	Quantification of 3 illegal additives: ADA, talcum powder, and gypsum powder	SGS, MSC, SNV	SVM, PLSR, BiPLS-IBPSO, CARS-IBPSO	R_V^2= 0.9786 (ADA); 0.9102 (talcum powder); 0.9226 (gypsum powder)	(Dong et al., 2024)
	Wheat Kernel and Flour	288	NIR	950-1650 nm	Discrimination of geographical origin of wheat kernel and flour with 3 genotypes across 4 years procured from 3 different areas of China	SNV, SGD	PCA, LDA	*Wheat Kernel* Accuracy: 61.1- 100% (geographical origin); 63,4% (production years); 98,2% (genotypes) *White Flour* Accuracy: 80.6%- 100% (geographical origin); 73% (production years); 86.1% (genotypes)	(Wadood et al., 2019)
	Wheat Flour	170	NIR	900-1700 nm	Quantification of four derived from the two registered local cultivars	BC, DT, MSC, SNV, SGS	PCA, PLSR	R_P^2= 0.965; RMSEP= 5.561% and RPD= 5.292	(España-Fariñas et al., 2025)
Monitoring the origin (traceability)	Wheat Flour	200	FT-MIR	4000-400 cm^{-1}	Classification of Iranian wheat flour varieties	SGD, SNV, MSC	PCA, SVM, LDA, ANN	Accuracy: 100% classification	(Fattahi et al., 2024)
	Wheat Grain	925	Vis-NIR, SWIR	Vis-NIR:400-1000 nm SWIR:950-2500 nm	Identification of 37 wheat varieties	SNV, SGD,	SVM, LDA	*Bulk samples* Accuracy: 93.72% (cross-validation); 94.93% (test sets) *Single kernels* Accuracy: 100% (cross-validation and test sets)	(Özdoğan & Gowen, 2025b)
	Wheat Flour	150	NIR-HSI	900-1700 nm	Detection of adulteration in Irish organic wheat flour (OWF) with common wheat flour (WF), cassava flour (CaF) and corn flour (CoF)	SGD, SNV	PLSR, PCR	R_P^2 = 0.986, 0.973 0.971 (CaF, CoF and WF, respectively) RMSEP=0.026, 0.036 and 0.038 (CaF, CoF and WF, respectively)	(Su & Sun, 2017)
	Durum Wheat Pasta	361	FT-NIR	10,000-4000 cm^{-1}	Authentication of Italian pasta made exclusively with durum wheat cultivated in Italy.	SVM, MC	PCA, PC-LDA, PLS-DA, SVM	Sensitivity: 95%; specificity: 94% Accuracy: 94%	(De Girolamo, Cervellieri, et al., 2020)

ADA: azodicarbonamide; ANN: artificial neural network; BC: Baseline correction; BiPLS-IBPSO: backward interval partial least squares combined with improved binary particle swarm optimization; BPO: benzoyl peroxide; BPNN: back propagation neural network; CARS-IBPSO: competitive adaptive reweighted sampling integrated with improved binary particle swarm optimization; DT: Detrending; FTIR: Fourier-transform infrared spectroscopy; GLSW: generalized least squares weighting; iSPA-PLS: successive projections algorithm for interval selection in partial least squares; MC: MC: mean centering; MSC: multiplicative scatter correction; N: number of samples; NIR: near infrared spectroscopy; NIR-HSI: near-infrared hyperspectral imaging; MIR: mid infrared spectroscopy; OFF: offset correction; PCA: principal component analysis; PCR: principal component regression; PLSR: partial least squares regression; RBF-NN: Radial Basis Function Neural Network; RMSECV: root mean square error of cross-validation; RMSEP: root mean square error of prediction; RPD: ratio performance to deviation for prediction; RS: Raman spectroscopy; SCM: Spectral Correlation Measurement; SGD: Derivate Savitzky–Golay derivate; SGS: Derivate Savitzky–Golay smoothing; SIMCA: Soft independent modeling by class analogy; SPA-MLR: successive projections algorithm for variable selection in multiple linear regression; SVM: support vector machine; SWIR: short-wave infrared food safety (Neill et al., 2012; Nisar et al., 2020). In this regard, Fu et al. (2020) and Fu et al. (2021) demonstrated the applicability of NIR hyperspectral imaging (NIR-HSI) for discriminating talc adulteration at concentrations as low as 0.02% (w/w), although clearer detection patterns were observed from 0.2% onwards. More recently, Shi et al. (2023) applied NIR spectroscopy combined with key wavelength selection algorithms, achieving robust predictive models for talc and BPO in the range of approximately 0.5% (w/w) and above. The results obtained demonstrate that NIR technology has the potential to discriminate the accurately predict the level of these two chemical additives in wheat flour, with detection limits as low as 0.02–0.5% (w/w), depending on the technique and model used, in a rapid and non-destructive manner. Dong et al. (2024) developed a method based on NIR spectroscopy combined with chemometric techniques for the rapid identification and detection of three illegal additives in wheat flour: azodicarbonamide (ADA), talcum powder, and gypsum powder. The PLSR model based on competitive adaptive reweighted sampling integrated with improved binary particle swarm optimization (CARS-IBPSO) achieved the best performance, with R^2_p values of 0.9786, 0.9102, and 0.9226 and RMSEP values of 0.0024%, 1.3693%, and 1.6506% for ADA, talcum powder, and gypsum powder, respectively. Notably, the method demonstrated the ability to detect ADA at concentrations as low as 0.002% (w/w), and talcum and gypsum powder from 0.25% (w/w) upwards.

Determining the geographical origin of food products is also a crucial factor to ensure quality of food products (Cozzolino, 2014). Consumers are increasingly interested in foods that are distinctly associated with a specific place of origin. A verified and guaranteed geographical origin often warrants a higher price, thus incorrect labeling is detrimental to both producers and consumers (Luykx & van Ruth, 2008). In the case of wheat, identifying the variety is an important topic discussed in recent literature. Additionally, the growing demand for organic foods highlights the need for the authenticity of organic wheat (H.-Y. Liu et al., 2023; Su & Sun, 2016).

Wadood et al. (2019) evaluated the suitability of using NIR reflectance spectroscopy in the 950–1650 nm range couple with chemometrics to classify wheat grain and flour according to origin, production year, and genotypes. Three genotypes were analyzed over four years and from three different geographical areas in China, applying PCA and LDA. The best results were obtained for the wheat flour matrix, with 100% accuracy for geographical origin and 73% for production years, while the wheat whole kernel showed a better classification percentage (98.2%) for genotypes. The study also highlighted that environmental conditions and genotype leave chemical signatures detectable in the NIR spectra, supporting the traceability of wheat. Recently, España-Fariñas et al. (2025) demonstrated the use of NIR spectroscopy combined with chemometrics to differentiate local wheat cultivars in PGI "Galician bread." From 160 flour mixtures containing varying proportions of *Caaveiro* and *Callobre*, the optimal PLSR model with detrending and multiplicative scatter correction achieved high predictive accuracy (R^2_p = 0.965, RMSEP = 5.561%, RPD = 5.292). Fattahi et al. (2024) studied the use of FT-MIR spectroscopy combined with chemometric methods to classify different varieties of wheat flour from Iran. Successful discrimination of flour varieties was achieved using LDA, SVM, and ANN models with the SGD + SNV preprocessing technique. The results show a classification accuracy of 100%. In particular, SVM and ANN clearly outperformed LDA, reaching 100% sensitivity and specificity in the test datasets without any misclassification. In a similar way, Özdoğan and Gowen (2025b) explored the potential of Vis-NIR and Short-Wave Infrared (SWIR) hyperspectral imaging for the automatic identification of thirty-seven wheat classes. Results showed that Vis-NIR achieved higher accuracy than SWIR. The best classification accuracy for single kernels was obtained with an LDA-SNV model using vertically and horizontally concatenated Vis-NIR and SWIR data, achieving 93.72% and 94.93% in 10-fold cross-validation and test sets, respectively. Bulk samples demonstrated superior classification performance, reaching 100% accuracy in both validation and test sets.

On the other hand, in addition to the importance of distinguishing durum wheat from common wheat, as previously mentioned, the geographical origin of the durum wheat used in pasta production is also an important factor. Thus, the objective of the study of De Girolamo et al. (2020b) was to apply FT-NIR and FT-MIR spectroscopy combined with chemometrics to authenticate Italian pasta made exclusively with durum wheat grown in Italy. Classification models were tested using both a three-class scheme (≤1%, 1–5%, >5%) and a two-class scheme with a 2% cut-off. The best performance was observed in the NIR range using the two-class scheme, achieving validation accuracies of 95–97%, whereas the three-class approach yielded slightly lower accuracies (89–95% in NIR and 80–90% in MIR).

At the same time, authentication of organic products is necessary due to frequent adulteration. For this purpose, Su and Sun (2017) evaluated the effectiveness of a hyperspectral imaging system to quantitatively detect adulteration of Irish organic wheat flour with soft wheat flour, cassava flour, and corn flour. For quantitative analysis, they employed PLSR and PCR. The R^2_P of the PLSR models (based on full spectrum and optimal wavelengths) were 0.971, 0.973, and 0.986 for wheat, corn, and cassava flour, respectively. The results obtained indicate that this method has the potential to authenticate wheat flour blends in the range of 3 to 75% (w/w %).

Despite the high classification accuracies frequently reported, many authentication studies rely on limited and well-controlled sample sets. The use of complex models combined with internal validation may increase the risk of overfitting, while external validation and model transferability across instruments, harvest years, and cultivars are still limited.

4.2. Evaluation of quality parameters

4.2.1. Chemical composition analysis

Another application of NIR and MIR spectroscopic techniques is the analysis of the chemical composition of flour and wheat-based products, as shown in Table 3, which is directly related to their nutritional quality and processing properties (Javid Iqbal et al., 2022).

The protein content, which normal variation ranges between 8% and 16%, is one of the main quality parameters of wheat (Goel et al., 2021). Consequently, methods based on spectral techniques have attracted significant research interest, as in the study of Huan et al. (2021) where the authors verified the capability of NIR for the quantitative detection of protein in wheat grains. For this purpose, AWVCPA algorithm was used to select characteristic wavelengths and reduce the model complexity, decreasing the number of spectral variables from 256 to only 10. PLSR was employed to build quantitative detection models. The selected wavelengths were mainly located around 1006 nm (second overtone of N–H stretching), 1203 nm (second overtone of C–H stretching), and 1478 nm (first overtone of N–H stretching), all closely related to amino acids and protein absorption. The results obtained with the AWVCPA-PLSR prediction model indicated high accuracy, with R^2=0.9753, RMSEP=0.0934, RPD=10.15, and RER=38.54.

Wheat flour crude protein content prediction was also evaluated to achieve a spectral standardization method between different NIR spectrometers (Tian et al., 2022). The crude protein content was measured with a S450 NIR spectrometer (master) and three N500 NIR spectrometers (target). The master PLS model reached high accuracy (Rc = 0.97, Rp = 0.96, RMSEP = 0.43, RPD = 4.22), but prediction performance dropped markedly when models were transferred without correction. After standardization using three algorithms (DS, PDS and SLRDS), the spectral difference between the spectrometers was significantly reduced, and the prediction effect of the PLS model was improved, with the DS algorithm showing the best results (Rp > 0.90, RMSEP < 1.0, RPD up to 3.16). Therefore, it can be concluded that the use of algorithms allows for the reduction of spectral differences between instruments, enabling the sharing of NIR calibration models for measuring crude protein in wheat flour. Recently, NIR and ATR-FT/MIR spectroscopy techniques

Table 3
An overview of infrared techniques application in chemical composition analysis of wheat flour and wheat-based products.

Sample	N	Technique	Spectral Range	Objective	Chemometrics			Reference
					Pretreatment	Model	Performance	
Wheat Grain	66	NIR	950-1690 nm	Quantification of protein content	None	PLSR,	R^2=0.9753; RMSEP=0.0934; RPD=10.15	(Huan et al., 2021)
Wheat Flour	34	NIR	800-2800 nm	Prediction of protein content	None	PCR, PLSR, PSCM	R^2= 0.9 for validation	(Ranzan et al., 2014)
Wheat Flour	154	NIR	S450: 900-2500 nm N500: 1550-1950 nm	Standardization methods between different NIR spectrometers in a crude protein model	SNV, Normalization, MSC, SGD	PLSR	R^2_P=0.9753; RMSEP=0.43; RPD=4.22	(Tian et al., 2022)
Wheat Flour	48	NIR, FTIR	NIR: 680-2500 nm FTIR: 4000-700 cm^{-1}	Determination of CP and IPD	MSC, SGD, SNV, DT	PLSR	**CP** (NIR): R^2=0.98; (FTIR): R^2=0.96 **IPD** (NIR): R^2=0.68; (FTIR): R^2=0.67	(Shi et al., 2019)
Wheat Flour	519	NIR	400-2500 nm	Determination of protein and moisture content	None	LGAKNet	R^2=0.9653 (protein); 0.9683 (moisture) RMSE=0.2886 g/100g (protein); 0.3061 g/100g (moisture) RPD=5.8981 (protein);5.1046 (moisture)	Yang et al. (2025)
Wheat Flour	376	FT-NIR	866-2534 nm	Prediction of gluten, gliadin, glutenin, ALGL, HMW-GS, LMW-GS	SNV, SGD	PLSR	RMSEP=2.01 mg/g (ALGL); 6.09 mg/g (gluten); 4.25 mg/g (gliadin); 3.50 mg/g (glutenin); 1.12 mg/g (HMW-GS); 2.38 mg/g (LMW-GS)	(Schuster et al., 2023)
Wheat Grain and Flour	25 (grain), 17 (flour)	NIR	1375-2500 nm	Prediction of protein, moisture and ash content	MSC, SGD	FCM, PLSR	**Wheat Grain** (FCM): RMSE= 0.581 (protein); 0.412 (moisture) (PLSR): RMSE= 0.65 (protein); 1.93 (moisture) **Wheat Flour** (FCM): RMSE= 1.06 (protein); 0.09 (moisture); 0.02 (ash) (PLSR): RMSE= 2.40 (protein); 0.38 (moisture); 0.055 (ash)	(Boglou et al., 2023)
Wheat Grain	48	NIR	320- 1100 nm	Prediction of protein and moisture content	None	ANN	R^2>0.99 RMSE= 0.4866% (protein); 0.2161% (moisture)	(Liu et al., 2022)
Wheat Grain	64	NIR, ATR-MIR	NIR: 950-1650 nm MIR: 4000-525 cm^{-1}	Determination of the RS content	GFS, MSC, MN, SGSG	PLSR	(NIR): R^2_C=0.672; R^2_P=0.552; RMSEC = 0.385; RMSEP = 0.459; RPD = 1.464 (MIR): R^2_C=0.927; R^2_P=0.828; RMSEC = 0.153; RMSEP = 0.284; RPD = 2.366	(Wang et al., 2021)
Wheat Grain, Wheat Bran, other cereals	396	FT-NIR	400-2500 nm	Determination of arabinose, xylose, glucose, cellulose, lignin, TS, RDS and SDS content	SNV, DT	mPLSR	R^2>0.97 (arabinose, xylose, and glucose); R^2=0.94 (lignin); R^2=0.70 (cellulose); R^2=0.99 (TS); R^2=0.81 (RDS and SDS)	(Nieto-Ortega et al., 2022)
Industrial Pastries, Biscuits	24 (pastries), 14 (biscuits)	Vis-NIR	350-2500 nm	Determination of proteins, moisture, fat, carbohydrates, as well as saturated, polyunsaturated and monounsaturated fats	MN, SGD	PCA, PLSR	R^2=0.928 and 0.964 (intact and ground pastry, respectively) R^2= 0.965 and 0.924 (intact and ground biscuits, respectively)	(Cayuela-Sánchez et al., 2020)
Wheat Bran	44	FT-NIR, ATR-FTIR	FT-NIR: 12,400 -4000 cm^{-1}	Determination of water, protein, ash, starch, SDF, IDF and lipids content	SGD	PLSR	(NIR): R^2=0.75 (water); 0.7 (protein); 0.88 (ash); 0.83 (starch); 0.77 (SDF);	(Hell et al., 2016)

(*continued on next page*)

Table 3 (*continued*)

Sample	N	Technique	Spectral Range	Objective	Chemometrics			Reference
					Pretreatment	Model	Performance	
			ATR-FTIR: 4000-550cm^{-1}				0.90 (IDF); 0.82 (lipids) (MIR): R^2=0.50 (water); 0.37 (protein); 0.78 (ash); 0.63 (starch); 0.29 (SDF); 0.74 (IDF); 0.65 (lipids)	
Wheat Flour	150 (protein), 239 (moisture), 192 (wet gluten), 160 (ash), 124 (sedimentation)	NIR	Spectral Engines NR 2.0-W: 1550-1950 nm Viavi MicroNIR: 908-1676 nm Si-Ware Systems: 1298-2606 nm	Suitability of 3 NIR spectrometers for the quantitative analysis of protein, wet gluten, moisture, ash, and sedimentation	SGD, SNV	PLSR	**Si-Ware** R_P^2=0.9488 (protein); 0.7079 (moisture); 0.9225 (ash); 0.8185 (sedimentation); 0.7874 (wet gluten) **Viavi** R_P^2=0.9422 (protein); 0.8175 (moisture); 0.9055 (ash); 0.7217 (sedimentation); 0.8585 (wet gluten) **Spectral Engines** R_P^2=0.8370 (protein); 0.6361 (moisture); 0.8106 (ash); 0.6309 (sedimentation); 0.6117 (wet gluten)	(Chen et al., 2021)
Wheat Bread	155	NIR	11,000-4000 cm^{-1}	Prediction of protein, moisture, ash, total gluten and dry gluten, as well as gluten index and falling number	SNV, SGD	PCA, PLSR	R^2= 0.99 (protein); 0.96 (moisture); 0.98 (ash); 0.98 (total gluten); 0.97 (dry gluten); 0.96 (gluten index); 0.97 (falling number) RPD= 9.63 (protein); 5.29 (moisture); 6.39 (ash); 8.09 (total gluten); 5.57 (dry gluten); 0.96 (gluten index); 6.23 (falling number)	(Abeshu & Kasahun, 2024)
Winter Wheat Grain	60	NIR	10,552- 390 cm^{-1}	Prediction of fertilization and crude protein concentration	SGD, SNV, MSC	PCA, PLSR	R^2= 0.98 (fertilization) and 0.98 (crude protein)	Von Wrochem et al. (2024)
Wheat Kernel	1440	Vis-NIR, SWIR	Vis-NIR: 400-1000 nm SWIR: 950-2500 nm		SGD, SNV, MSC	LDA, ANN	Accuracy: 85.24–94.35% (vitreous kernels); 72.24–83.83% (non-vitreous kernels)	(Özdoğan & Gowen, 2025a)
Wheat Flour fortified with Lentil Flour	153	NIR	1100-2000 nm	Prediction of mineral composition (Ca, Mg, Fe, K and P)	MSC, SNV, DT, SNV-DT	PCA, mPLSR	Correct classified: 100% (calibration data) and 96.67% (validation data)	(Martínez-Martín et al., 2023)
Wheat Kernel and Flour	631	Vis-NIR	375-1050 nm	Predicting of Ca, Mg, Mo and Zn	SGD, COE, VN, MMN, MSC	PLSR	Kernel: R^2=0.70 (Ca); 0.74 (Mg); 0.82 (Mo); 0.77 (Zn) Flour: R^2=0.48 (Ca); 0.72 (Mg); 0.77 (Mo); 0.63 (Zn)	(Hu et al., 2021)
Wheat Grain	402	Vis-NIR	400-1700 nm	Prediction of 422 nutrients	FD, SD	PLSR, LASSO, SLR	R2 > 0.6; RPD > 1.5	(Shi et al., 2024)
Wheat Flour	107	FT-NIR	10,000-4000 cm^{-1}	Rapid determination of TPC	MSC, SGD	PCA, PLSR	R^2= 0.92 (calibrations set); 0.90 (validation set)	(Tian et al., 2021)
Wheat Flour	120	NIR	899.22-1724 nm	Quantitative detection of fatty acid value during storage	SNV	ELM, PLSR	R_P^2>0.96	(Jiang et al., 2020)
Wheat Flour	8	FTIR	4000 - 800 cm^{-1}	Study of variations during storage through analytical and rheological parameters	BC	PCA, PLSR	R_{CV}^2=0.97; RMSECV=0.11 (crude protein) R_{CV}^2=0.88; RMSECV=0.41 (wet gluten content)	(Ahmad et al., 2022)
Wheat Flour and Bread	ND	FTIR	1400-800 cm^{-1}	Estimating of phytic acid during the bread-making process	None	MLR	R^2= 0.986	(Dave & Modi, 2018)

combined with chemometrics were compared as their performance to determine crude protein (CP) and intestinal protein digestibility (IPD) of wheat (Shi et al., 2019). The PLSR models generated for both techniques showed similar predictive capabilities for CP, with the best NIR model having an R^2=0.98 and the best MIR model having an R^2=0.96. Also, for IPD, the best NIR model had an R^2=0.68, and the best MIR model had an R^2=0.67. The CP content in wheat samples ranged from 11.88 to 20.03%, while IPD values varied between 67.23 and 83.22%, highlighting the broader accuracy of IR techniques for chemical composition compared to physiological traits. Key spectral regions included 2148–2200 nm in NIR and the amide I (~1650 cm^{-1}) and amide II (~1550 cm^{-1}) bands in MIR. These results demonstrate that IR spectroscopy allows for the determination of crude protein content, but further studies are needed to improve its performance in evaluating digestibility.

Recent studies have demonstrated the potential of NIR spectroscopy for real-time protein analysis in wheat flour. Yang et al. (2025) combined a lightweight deep learning algorithm (LGAKNet) with NIR spectroscopy to predict protein and moisture with high accuracy (protein: R^2 = 0.9653, RMSE = 0.2886 g/100 g; moisture: R^2 = 0.9683, RMSE = 0.3061 g/100 g). The system achieved a detection speed of ~7 samples per second, confirming its suitability for in-line quality monitoring.

Gluten proteins have a crucial impact on the quality and properties of wheat flour and its derivative products, such as bakery products and bread (Ma et al., 2019). Considering this, Schuster et al. (2023) explored the ability of NIR for gluten, gliadin and glutenin in wheat flour quantification and prediction of albumin/globulin (ALGL), high-molecular-weight glutenin subunits (HMW-GS) and low-molecular-weight glutenin subunits (LMW-GS) prediction. The concentration ranges analyzed were 48.18–124.53 mg/g for gluten, 25.86–70.03 mg/g for gliadins, 17.68–57.13 mg/g for glutenins, 2.62–14.18 mg/g for albumins/globulins (ALGL), 2.15–12.36 mg/g for high-molecular-weight glutenin subunits (HMW-GS), and 14.49–44.77 mg/g for low-molecular-weight glutenin subunits (LMW-GS). The PLSR models achieved prediction errors RMSEP of 6.09 mg/g (gluten), 4.25 mg/g (gliadin), 3.50 mg/g (glutenin), 2.01 mg/g (ALGL), 1.12 mg/g (HMW-GS), and 2.38 mg/g (LMW-GS). While the relative errors for ALGL, HMW-GS, and LMW-GS were too high for reliable quantification, the prediction performance for gluten, gliadins, and glutenins were comparable to the acceptable error of the reference RP-HPLC method. In addition, technologically important ratios such as gliadin/glutenin (0.88–2.28, RMSEP = 0.22) and LMW-GS/HMW-GS (2.22–9.10, RMSEP = 0.27) could be estimated with reasonable accuracy.

Boglou et al. (2023) employed a low-cost portable NIR spectrometer (NeoSpectra) combined with fuzzy cognitive maps (FCMs) to estimate protein, moisture, and ash contents in wheat grains and flour. The models showed R^2 values above 0.90 for both protein and moisture in wheat, with maximum deviations of only 1% from reference values, while no reliable model was reported for ash in grain. In flour (mean ≈0.58%), ash could be estimated ($R^2 < 0.90$; RMSEP = 0.020% for the FCM model and 0.055% for the PLS model), although with lower accuracy compared to protein and moisture. In this context, Liu et al. (2022) developed an artificial neural network method for predicting wheat grain quality based on moisture and protein content. The RMSE for wheat protein and moisture content were 0.4866 and 0.2161%, respectively, with $R^2 > 0.99$ for both, indicating that the developed method effectively provides information on wheat grain quality. Additionally, Abeshu and Kasahun (2024) developed a rapid and cost-effective method to evaluate major quality parameters of bread wheat grain using NIR. To achieve this, a total of 155 bread wheat samples were analyzed. The developed PLSR model demonstrated high predictive performance for key quality parameters, achieving R^2 values of 0.99 for protein, 0.96 for moisture and gluten index, 0.98 for ash and total gluten, and 0.97 for the falling number.

Nitrogen fertilization directly affects protein content and baking quality in wheat, but its use is also associated with environmental and economic concerns. Experimental studies addressing these effects, such as greenhouse pot experiments and field trials, are frequently limited by the small number of samples available, which complicates the development of robust calibration models. To address this challenge, Von Wrochem et al. (2024) investigated the applicability of NIR spectroscopy to predict protein content and related traits under reduced nitrogen fertilization using restricted experimental datasets. Two winter wheat cultivars (Discus and Rumor) were grown under different late nitrogen fertilization regimes and analyzed through NIR spectroscopy. The spectral data enabled discrimination of fertilization levels, cultivars, and growing conditions, with specific bands related to gluten and starch showing clear variation. PLSR models achieved very high predictive performance for crude protein in Discus (R^2 = 0.98) and acceptable results in Rumor (R^2 = 0.83). Authors pointed out that the model performance was cultivar-specific and not directly transferable.

Vitreousness of wheat kernels, a property associated with endosperm compaction, grain hardness, protein content, and end-use quality, was analyzed by hyperspectral imaging in the study of (Özdoğan & Gowen, 2025a). The best performance was obtained in the Vis-NIR region with SVM combined with Savitzky–Golay first derivative preprocessing, reaching 90.28% accuracy in cross-validation and 89.35% in the test set. Vitreous kernels were classified more accurately (specificity 85.24–94.35%) than non-vitreous kernels (sensitivity 72.24–83.83%).

On the other hand, carbohydrates are the main components of cereals (70-80%) (Slafer et al., 2021). Therefore, spectral techniques have been studied for determining their content, as demonstrated in the study by Nieto-Ortega et al. (2022). In this work, the authors evaluated the capability of NIR reflectance spectroscopy technology to predict the content of arabinose, xylose, glucose, cellulose, lignin, and total starch, as well as rapidly (RDS) and slowly (SDS) digestible starch in various cereals, including wheat and wheat bran. They employed the modified PLSR (mPLSR) method, through which they achieved a strong correlation between the NIR spectra obtained and the reference data. The developed NIR calibrations provided accurate predictions for all parameters, with R^2 values above 0.97 and RPD > 5.0 for arabinose, xylose, glucose, lignin and total starch (12.2–69.2 g/100 g), while cellulose showed moderate predictability (R^2 = 0.70). In addition, starch digestibility fractions were successfully estimated, with R^2 = 0.81 for RDS (8.2–28.7 g/100 g) and R^2 = 0.95 for SDS (0.1–45.0 g/100 g). In addition, other studies have also applied NIR combined with PLSR to simultaneously evaluate proteins, moisture, ash, fats, and carbohydrates in industrial pastries and biscuits (Cayuela-Sánchez et al., 2020), wheat bran (Hell et al., 2016), and wheat flour (Chen et al., 2021).

Wang et al. (2021) compared the effectiveness of NIR and ATR-MIR spectroscopy with the PLSR algorithm for determining the resistant starch (RS) content in wheat grains. The ATR-MIR calibration clearly outperformed NIR, achieving R^2_c = 0.937 and R^2_p = 0.828 with an RMSEP of 0.284 and RPD = 2.37, while the NIR model showed weaker predictive performance (R^2_p = 0.552, RMSEP = 0.459, RPD = 1.46). External validation further confirmed the superiority of ATR-MIR (R^2 = 0.919) compared to NIR (R^2 = 0.773). Importantly, the ATR-MIR model was applied to screen 1010 wheat mutant lines, enabling the rapid identification of two high-RS mutants (≈2.55% and 2.12%). The authors also highlighted that the total time required for the measurement of each sample was less than 5 minutes, compared to approximately 20 hours needed for chemical determination of RS content. The validation of the optimal calibration models developed for NIR and ATR-MIR demonstrated that the ATR-MIR model outperformed the NIR model in predicting RS content.

Apart from the primary chemical composition attributes, spectroscopic techniques were also utilized to examine the determination of total phenolic content, mineral composition, fatty acids, and phytic acid in wheat. Due to the numerous health benefits provided by phenolic compounds in wheat, developing a method for the rapid detection of total phenolic content (TPC) is of great interest. For this objective, Tian

Table 4
An overview of infrared techniques application in technological parameters analysis of wheat flour and wheat-based products.

Sample	N	Technique	Spectral Range	Objective	Chemometrics			Reference
					Pretreatment	Model	Performance	
Durum Wheat	9	FTIR	4000- 600 cm^{-1}	Measurement of rheological properties	SGD	PLSR	R^2= 0.832 (for strength of the network structure)	(Fanari et al., 2022)
Wheat Flour	1028	NIR	850-1650 nm	Prediction of farinograph characteristics: water absorption (a), dough development time (b), dough stability (c) and degree of softening (c)	SNV, DT, MSC, SGD	PLSR, PCR, GPR	R^2= 0.908 (a); 0.772 (b); 0.827 (c); 0.818 (d) (training dataset) R^2= 0.817 (a); 0.704 (b); 0.788 (c); 0.766 (d) (test dataset)	(Cui et al., 2023)
Wheat Bread Loaves	677	NIR	900-1670 nm	Determination of the fermentation state	SGD, SNV, MC	PLSR-DA	Sensitivity= 88% (unfermented dough); 86% (fermented and over-fermented doug) Specificity> 86% (all cases)	(Castro-Reigía et al., 2024)
Wheat Grain	1200	NIR, Raman, Fluorescence	12,500-3600 cm^{-1}	Determination of 73 wheat quality parameters	Different pre-processing methodologies	PLSR	R^2= 0.95 (protein content); 0.839 (sedimentation volume); 0.659 (baking behavior); 0.755–0.823 (water absorption); 0.87(extensibility); 0.94 (resistance to extension); 0.95 (energy)	(Nagel-Held et al., 2024)
Wheat Bread	1082	NIR	1000-1799 nm	Determination of farinograph and extensograph characteristics	DT, MA, WT, MSC, SGS	PLSR, SVR and CNN	R^2v = 0.90; RPD = 3.20 (farinograph water absorption) R^2v = 0.68–0.75 (extensograph characteristics)	(Zhao et al., 2025)
Wheat Grain	882	NIR	2,498-400 nm	Prediction of protein content, test weight, PSI, water absorption, dough development time and mixing tolerance index	SNV, SGD, Smoothing,	ANN, RF, PLSR	R^2= 0.988 (protein content); 0.756 (test weight); 0.826 (PSI); 0.914 (water absorption); 0.581 (dough development time); 0.972 (mixing tolerance index)	(Williams, 2020)
Wheat Flour	921 (SV), 904 (FN)	NIR	900-1700 nm	Prediction of SV and FN	None	PCA, SOA-SVR	R_P = 0.9752 (SV); 0.9497 (FN) RMSEP = 0.2138 (SV); 0.2930 (FN)	(Wang et al., 2025a)
Wheat Flour	154	NIR, FT-NIR	NIR: 400 -2500 nm (reflectance), 800- 1000 nm (transmission) FT-NIR:1350-2500 nm	Prediction of loaf volume	SGD, MSC	PCA, PLSR	$R^2 \approx$ 0.85–0.88; RMSEP $\approx$ 124–126 cm^3 (NIR) $R^2 \approx$ 0.80; RMSEP $\approx$ 138 cm^3 (FT-NIR)	(Czaja et al., 2025)
Wheat Flour	1500	NIR	900-1700 nm	Prediction of dry and wet gluten content and gluten index	SGS. SNV, MSC, Normalization	SVR	R_P = 0.9370-0.9430; RMSEP = 0.3450-0.4043%, and RPD = 3.1348-3.4998)	(Wang et al., 2025b)
Wheat Flour	70	ATR-FTIR	4000- 650 cm^{-1}	Determination of moisture, ash, protein, wet gluten, sedimentation index, pH, acidity, fat, starch, falling number, damage starch and glutograph parameters stretching and relaxation	BC, Normalization, SGD, SNV, MSC	PCA, PLSR	R^2_C > 0.964and R^2_V> 0.749	(Golea et al., 2023)

ANN: artificial neural networks; ATR: Attenuated total reflection; BC: baseline correction; CNN: convolutional neural networks; DT: detrending; FN: falling number; FTIR: fourier-transform infrared spectroscopy; GPR: Gaussian process regression; MA: moving average; MC: mean centering; MSC: multiplicative scatter correction; N: number of samples; NIR: near infrared spectroscopy; PCA: principal component analysis; PCR: principal component regression; PLSR: partial least squares regression; PLSR-DA: partial least squares regression- discriminant analysis; PSI: particle size index ; SGD: Savitzky–Golay derivation; SGS: Savitzky–Golay smoothing; SOA- SVR: starfish-optimization-algorithm-optimized support vector regression; SV: sedimentation value; SVR: support vector regression; RF: random forest; WT: wavelet transform.

et al. (2021) investigated a PLS regression model based on NIR spectroscopy for rapid determination of total phenolic content of whole wheat flour. The optimal regression model showed high predictive accuracy for whole wheat flour TPC with R^2 values of 0.92 and 0.90 for the calibration and validation sets, respectively. In a recent work, Martínez-Martín et al. (2023) used NIR technology for determination of prediction of mineral composition (Ca, Mg, Fe, K and P) in wheat flours fortified with lentil flour. The results obtained with the developed MPLS models allow them to conclude that it is possible to discriminate fortified flours with 100% efficiency and determine their mineral content. In particular, prediction models achieved excellent performance for K (0.016–1.34 g/100 g, $R^2 = 0.98$), Mg (0.015–0.14 g/100 g, $R^2 = 0.96$), P (0.018–0.56 g/100 g, $R^2 = 0.94$), and Ca (0.005–0.13 g/100 g, $R^2 = 0.94$), while Fe was predicted with slightly lower accuracy (10.6–115 mg/kg, $R^2 = 0.87$). External validation confirmed the robustness of these models, with no significant differences compared to ICP-MS reference values. Similarly, Hu et al. (2021) managed to predict Ca, Mg, Mo, and Zn nutrients in wheat kernel and flour using Vis-NIR technology in combination with chemometrics, with R^2 values of 0.70 for Ca, 0.74 for Mg, 0.82 for Mo, and 0.77 for Zn in kernels, while in flour the prediction ability decreased ($R^2 = 0.72$ for Mg, 0.77 for Mo, and 0.63 for Zn). The results obtained for the optimal PLSR model showed high accuracy, although higher in wheat grains than in flour. When considered alongside the study of Martínez-Martín et al. (2023), which reported higher calibration performance for several minerals (K, P, Mg, Ca) in fortified wheat flours ($R^2 > 0.94$), it can be inferred that Vis-NIR hyperspectral imaging may be advantageous for simultaneously screening a broader range of micronutrients, while conventional NIR spectroscopy appears to offer more robust quantification for specific minerals under certain experimental conditions.

Additionally, in a recent study, Shi et al. (2024) developed a high-throughput method for the non-destructive quantification of hundreds of nutrients in wheat grains using VIS-NIR hyperspectral imaging (400-1700 nm) combined with deep learning techniques. A total of 402 wheat accessions were analyzed, leading to the identification of 422 metabolites, including amino acids and their derivatives, flavonoids, lipids, polyphenols, nucleic acids and their derivatives, organic acids and sugars, phenolamides, mineral elements, and vitamins. Different regression algorithms were evaluated (PLSR, LASSO, and SLR), and the stepwise linear regression model with first derivative preprocessing (SLR-dA) provided the best results. Using this approach, 220 nutrients were accurately predicted with $R^2 > 0.6$, and 77% of them achieved RPD values above 1.5, indicating robust predictive performance. The highest accuracies were obtained for several lipids (linolenic acid, $R^2 = 0.91$), amino acids and derivatives (melatonin, $R^2 = 0.75$), polyphenols (vanillin, $R^2 = 0.77$), and minerals such as Mg, Fe, Ni, Cu, Zn, and Mo, which all exceeded $R^2 = 0.7$.

During grain storage, significant changes occur in the lipid profile, which is an important factor in determining wheat flour quality (Lancelot et al., 2021). Jiang et al. (2020) used portable NIR equipment to quantitatively determine the changes in fatty acids of wheat flour during storage. Predictive models were built using an Extreme Learning Machine (ELM), demonstrating good and robust predictive accuracy. In this study, 120 wheat flour samples stored for up to six months at 25 °C were analyzed, with fatty acid values ranging from 30.2 to 47.5 mg KOH/100 g. The best ELM models, developed after wavelength selection with Variable Combination Population Analysis (VCPA), achieved R^2 values above 0.96 with RMSEP around 0.9 mg KOH/100 g, showing similar performance to optimized PLS models ($R^2 = 0.97$). The most informative spectral regions were located around 1562–1564 nm and 1103 nm, associated with C–H overtone vibrations of fatty acids. Ahmad et al. (2022) evaluated variations during storage in wheat flour using FTIR combined with chemometric tools such as PCA and PLSR to analyze both analytical and rheological parameters. The PLSR prediction models only demonstrated high accuracy in estimating crude protein and wet gluten content, with $R^2_{CV} = 0.97$ and 0.88, respectively. Moderate prediction ability was achieved for moisture ($R^2CV = 0.72$), fat (0.70), and ash (0.66), whereas fiber (0.54) and farinograph parameters (≤ 0.61) showed limited predictability. Spectral variations were mainly observed in protein-related bands (Amide I and II) and OH regions associated with moisture, and PCA enabled clear discrimination of flour samples according to storage time, particularly within the first three days.

FTIR has also been employed to estimate the content of phytic acid, a compound with adverse effects, during the bread-making process. Dave and Modi (2018) used MLR models based on FTIR spectroscopy for its determination and managed to develop a fast and sensitive method for its quantification, achieving a R^2 of 0.986. Characteristic absorption peaks of phytic acid were observed at 889, 1002, 1154, 1361 and 1418 cm^{-1}, corresponding to P–H and phosphate group vibrations. The method requires only ≈ 1 mg of sample mixed with KBr and less than 5 minutes of preparation time, making it faster and less laborious than conventional chemical methods such as ferric precipitation, HPLC, or AOAC 986.11.

Although strong predictive performance is commonly observed for major compositional parameters, many studies are based on relatively limited and homogeneous datasets and rely primarily on internal validation strategies. Consequently, the robustness of these models and their transferability under more variable production conditions remain insufficiently explored.

ATR: Attenuated total reflection; BC: baseline correction; COE: constant offset elimination; CP: intestinal crude protein; DT: detrending; ELM: extreme learning machine; FCMS: fuzzy cognitive map; FD: first derivate; FTIR: fourier-transform infrared spectroscopy; GFS: gaussian filter smoothing; HMW-GS: high-molecular-weight glutenin subunits; IDF: insoluble dietary fiber; IPD: intestinal protein digestibility; LASSO: Least absolute shrinkage and selection operator; LDA: linear discriminant analysis; LGAKNet: lightweight deep learning algorithm; LMW-GS: low-molecular-weight glutenin subunits; MMN: min–max normalization; MN: baseline mean normalization; MLR: multiple linear regression; MSC: multiplicative scatter correction; mPLSR: modified partial least squares regression; N: number of samples; ND: not determined; NIR: near infrared spectroscopy; MIR: mid infrared spectroscopy; PCA: principal component analysis; PLSR: partial least squares regression; PSCM: pure spectra components modeling; RDS: rapidly digestible starch; RS: resistant starch; SDF: soluble dietary fiber; SD: second derivate; SDS: slowly digestible starch; SLR Stepwise linear regression; SGS: Savitzky–Golay smoothing; TPC: total phenolic content; TS: total starch content; VN: vector normalization.

4.2.2. Technological parameters analysis

Evaluation of technological parameters of wheat is one of the main applications of spectroscopic techniques. Rheological properties include farinograph, mixograph, extensograph, and alveograph characteristics. They play an essential role in evaluating flour quality (Caporaso et al., 2018; Della Valle et al., 2022). Consequently, multiple non-destructive methods have been developed for their determination (Table 4)

Fanari et al. (2022), investigated the relationship between protein secondary structures and the rheological behavior of durum wheat dough using FTIR spectroscopy through indirect spectral measurements. Three semolina samples with different gluten quality were analyzed at various hydration levels, focusing on the Amide III region (1200–1340 cm^{-1}). They employed a PLS model along with the variable importance in projection (VIP) technique and, the weak gel model was applied to describe the gluten network. PLSR models demonstrated a good correlation between the Amide III band and the network strength parameter ($R^2 = 0.832$), with β-sheets and α-helices identified as the most influential structures, although correlations with the extension parameter were weaker ($R^2 = 0.550$).

Farinograph characteristics can estimate rheological properties and include water absorption, dough development time, dough stability, and degree of softening. Cui et al. (2023) used NIR spectroscopy to develop

Gaussian Process Regression–Partial Least Squares Regression (GPR-PLSR) model for farinograph properties (water absorption, dough development time, stability, and degree of softening) in wheat flour with protein contents ranging from 7 to 19%. NIR spectra (850–1650 nm) were preprocessed using SNV, MSC, detrending, and Savitzky–Golay derivatives. While conventional PLSR and PCR models performed reasonably well only for water absorption ($R^2 \approx 0.86$), their accuracy was poor for the other parameters ($R^2 < 0.38$). In contrast, the GPR-PLSR approach substantially improved predictive performance, achieving $R^2 = 0.817$ (RMSEP = 1.89, RPD = 3.19) for water absorption, $R^2 = 0.704$ (RMSEP = 1.62, RPD = 2.30) for development time, $R^2 = 0.788$ (RMSEP = 2.42, RPD = 2.28) for stability, and $R^2 = 0.766$ (RMSEP = 15.03, RPD = 2.00) for degree of softening.

On the other hand, Castro-Reigía et al. (2024) developed an efficient methodology to monitor bread fermentation process of bread dough in the baking industry using NIR combined with partial least squares discriminant analysis (PLS-DA). The proposed methodology accurately identifies the optimal fermentation point, preventing the baking of improperly fermented dough and reducing production costs. The results showed that the sensitivity for unfermented dough was 88%, while for fermented and over-fermented dough, it was 86%; specificities were above 86% in all cases.

In a recent work, Nagel-Held et al. (2024) investigated the ability of NIR spectroscopy to evaluate a wide range of 73 quality parameters associated with wheat. These researchers aimed to analyze various parameters, such as nutritional content, milling characteristics, gluten strength, dough properties and baking performance. The results from the optimal PLSR models showed high prediction accuracy for several technological properties. Water absorption was predicted with high reliability ($R^2 = 0.823$, RMSECV $\approx$ 1.0 mL/100 g), outperforming Raman and fluorescence models. Extensibility also showed moderate predictive power ($R^2 = 0.736$, RMSECV = 13.7 mm), while among GlutoPeak parameters, maximum torque reached acceptable accuracy ($R^2 = 0.763$). In contrast, other farinograph and rheological traits, as well as baking loss, could not be reliably predicted using NIR. Similar results have been observed by Zhao et al. (2025), who calibrated NIR models with more than one thousand wheat samples. They reported excellent predictive accuracy for farinograph water absorption ($R^2v = 0.90$, RPD = 3.20), while extensograph traits such as energy, extensibility, and maximum resistance reached moderate accuracy (R^2v = 0.68–0.75). Results suggested that while the technique is robust for certain key properties, its performance remains limited for more complex technological attributes,

In the same context, Williams (2020) studied the suitability of various algorithms for processing NIR spectral data in predicting several quality factors of wheat, such as protein content, test weight, particle size index, water absorption, dough development time, and mixing tolerance index. The algorithms used were artificial neural networks (ANN), support vector regression least squares support vector machines (SVR-LSSVM), and random forest (RF). The results demonstrated high prediction accuracy for all parameters (e.g., water absorption $R^2 = 0.93$, RPD = 3.6; the mixing tolerance index $R^2 = 0.94$, RPD = 4.1 and alveograph W value, representing dough strength, $R^2 = 0.98$, RPD = 6.4). except farinograph development time with the Random Forest algorithm, although all methods successfully predicted the protein content.

Recent studies have tested and validated miniaturized NIR systems for on-site evaluation of technological properties in wheat flour. Wang et al. (2025a) showed that a portable NIR spectrometer (900–1700 nm) combined with support vector regression optimized by the starfish optimization algorithm (SOA-SVR) could accurately predict sedimentation value (SV) and falling number (FN). Their models achieved excellent predictive performance with full spectra (SV: RP = 0.9752, RMSEP = 0.2138 mL; FN: RP = 0.9497, RMSEP = 0.2930), while wavelength reduction preserved accuracy despite eliminating over 90% of the variables. Similarly, Czaja et al. (2025) demonstrated that portable NIR devices can also predict white bread loaf volume, a key indicator of baking performance. Using both benchtop and handheld FT-NIR spectrometers, they reported high prediction accuracies, with the benchtop systems reaching the best performance ($R^2 \approx$ 0.85–0.88; RMSEP $\approx$ 124–126 cm^3) and the portable instrument still delivering reliable results ($R^2 \approx 0.80$; RMSEP $\approx$ 138 cm^3).Wang et al. (2025b) applied a miniaturized NIR device to quantify gluten quality parameters, including dry and wet gluten content and gluten index, achieving high prediction accuracies with SVR models (RP = 0.937–0.944; RPD = 3.13–3.50). Together, these findings confirm that portable NIR systems enable much faster on-site analysis of flour quality.

Golea et al. (2023) investigated FTIR application for quality control prediction in wheat flour. For this purpose, they analyzed and measured moisture, ash, protein, wet gluten, fat, starch, acidity, sedimentation index, falling number, damaged starch, and stretching and relaxation parameters. Through FTIR spectral analysis and chemometric techniques, robust PLSR models were established with $R^2_C > 0.964$ and $R^2_V > 0.749$, enabling precise quantification and characterization of wheat flour quality.

Thus, technological parameters are influenced by multiple interacting factors related to raw material properties and processing conditions. While the reviewed studies report generally good predictive performance, most models are validated under specific experimental conditions. Consequently, the transferability of these models across different wheat varieties, processing conditions, and experimental settings remains insufficiently explored.

4.3. Safety analysis

Non-destructive detection methods have also been utilized in the mitigation of food contamination risk (Sindhu & Manickavasagan, 2023) (Table 5). Continuing with this approach, Yin et al. (2021) investigated the use of NIR and computer vision (CV) to identify foreign contaminants, including metallic iron, polypropylene plastic, and hair, in terms of the minimum size of physical contaminants, in toast bread. The developed method exhibited high accuracy, identifying metallic fragments as small as 4 × 1 mm and 2 × 1 mm, plastic pieces down to 6 × 2 mm, and human hair with a diameter of approximately 70 μm and a length of 6–8 mm. In validation, the classification accuracy reached 97% for iron, 93% for plastic, and 91% for hair, making it a useful tool for detecting foreign contaminants in bread. In the same context, Kan et al. (2024) developed a method for the non-destructive detection of polystyrene microplastics in wheat flour using FT-NIR spectroscopy combined with chemometric techniques and a minimum detectable level of 100 mg of polystyrene microplastic/kg wheat flour. The developed PLSR models achieved $R^2_P = 0.9810$, RMSEP = 0.0462%, and RPD = 7.3890, highlighting the potential of FT-NIR spectroscopy as an effective and promising tool for quality control and food safety regarding microplastic contamination.

The identification of allergens is also a vital factor in minimizing contamination risks. Zhao et al. (2018) evaluated the use of NIR-HSI for the detection and prediction of peanut and nut powders in whole wheat flour. Using PLSR, individual models for each allergen achieved reliable quantification down to 0.5% (w/w), with high predictive accuracy ($R^2_P \approx 0.95$, RMSEP < 0.5%). In contrast, a combined model for both allergens showed reduced sensitivity, with a minimum detectable concentration of 1% (w/w) and lower predictive performance ($R^2_P \approx 0.90$, RMSEP $\approx$ 0.8%). For classification, PLS-DA successfully distinguished contaminated from uncontaminated samples at concentrations as low as 0.5% (w/w). Moreover, the real-time detection of gluten remains a necessity for the food industry. Thus, Adedeji et al. (2023) developed a method to detect and quantify wheat flour contamination in gluten-free bread using FTIR spectroscopy combined with machine learning techniques. The PLSR quantification models achieved R^2_P and RMSEP values of 0.99 and 0.34, respectively, allowing reliable quantification from concentrations as low as 0.5% (w/w). In addition, ensemble

Table 5
An overview of infrared techniques application in safety analysis of wheat flour and wheat-based products.

Sample	N	Technique	Spectral Range	Objective	Chemometrics			Reference
					Pretreatment	Model	Performance	
Toast Bread	320	NIR with CV	12,500-4000 cm^{-1}	Detection of metallic iron, polypropylene plastic, and hair	SGS, SGD	PCA, DA	Accuracy: 98% (metallic iron), 94% (polypropylene plastic) and 91% (hair)	(Yin et al., 2021)
Wheat Flour	120	FT-NIR	10,000-4000 cm^{-1}	Quantitative detection of polystyrene microplastics	SNV	PLSR	R_P^2=0.9810; RMSEP=0.0462%; RPD= 7.3890	(Kan et al., 2024)
Wheat Flour	19	NIR-HSI	936–1720 nm	Prediction of peanut and walnut powders	SNV, SGD, DT	PLSR	**Peanut** R_P^2=0.981–0.988; RMSEP=0.348–0.465 **Walnut** R^2_P= 0.990–0.997; RMSEP: 0.170–0.324 **Peanut + Walnut** R_P^2=0.960–0.987; RMSEP: 0.373–0.645	(Zhao et al., 2018)
Gluten-Free Bread	13	FTIR	4000-450 cm^{-1}	Detection of wheat flour contamination	SC, standardization	PCA,	R_P^2=0.99; RMSEP=0.34	(Adedeji et al., 2023)
Wheat Kernel and Flour	143	Vis-NIR, MIR	Vis-NIR: 305-1700 nm MIR: 4000-650 cm^{-1}	Detection and prediction of FHB infection	SGS	RF, LDA	**Wheat Kernel** (Vis-NIR): accuracy: 98.2% (MIR): accuracy: 93.1 – 96.4% **Wheat Flour** (Vis-NIR): accuracy: 98.2-100% (MIR): accuracy: 98,2- 100%	(Almoujahed et al., 2024)
Wheat Kernel and Flour	95	Vis-NIR	400-1650 nm	Prediction and classification of DON contamination	SGS, Normalization	RFC, RFR, ETC, ETR, ABC, ABR	**Prediction** R^2 = 0.94; RMSEP = 3.42 mg.kg^{-1} **Classification** Accuracy: 89.5 %	(Almoujahed et al., 2025)
Wheat Kernel and Flour	96	Vis-NIR, SWIR	Vis-NIR: 400-1000 nm SWIR: 1000-2000 nm	Detection of DON	MSC, SNV	SVM, SAE	**Wheat Kernel** (Vis-NIR): accuracy: 100% **Wheat Flour** (SWIR): accuracy: 100% (training set) and 96% (test set)	(Liang et al., 2020)
Wheat Grain	557	NIR	900–1700 nm	Detection of early asymptomatic FHB	SGS, SGD, SNV, MSC	RF, XGB, SVM	Accuracy: 73.33%	(Ba et al., 2023)
Wheat Kernel	300	NIR-HSI	895–1728 nm	Fusarium damage detection and DON prediction	SGD, MSC, SNV, BC, Normalization	PLSR, LDA, K-NN, ANN	R^2=0.88; RMSEP=6.65; RPD=3.21 Accuracy: 85.8% (fungal symptoms) and 76.9% (DON) at the EU limit	(Femenias et al., 2022)
Wheat Kernel	240	NIR-HIS	900-1700 nm	Detection of FD and DON contamination	None	K-NN	Accuracy: 85% (FD) and 80% (DON) Sensitivity: 92% (FD) and 77% (DON)	(Nadimi et al., 2021)
Wheat Grain	100	NIR	900-1630 nm	Quantification of ZEA	SGS, MSC, VN	PLSR, MLR	R_P^2=0.99; RMSEP=2.1 μg·kg^{-1}; RPD=6.0	(Ning et al., 2022)
Wheat Flour	267	FT-NIR	12,500-3600 cm^{-1}	Screening of DON contamination in	Smoothing, BC, normalization, MSC, SNV	PLSR-DA, PC-LDA	Accuracy: 85–87.5% (PLS-DA model) and 85% (PC-LDA model)	(Tyska et al., 2021)
Wheat Flour	195	Vis-NIR-HSI	363-1023 nm	Prediction and quantification of DON	Normalization	PCA, LDA, PLSR	R_P^2 = 0.691; RMSEP=0.707 μg·kg^{-1} Accuracy: 96.92%	(Zhao et al., 2020)
Wheat Kernel	ND	ATR-FTIR	4000-400 cm^{-1}	Prediction of DON contamination	SGD, SROI, EMSC	PCA, PLSR-DA	Accuracy of the cross validation: > 0.840	(Fomina et al., 2024)
Wheat Flour	196	NIR	901-1701 nm	Determination of ZEA	None	PCA, RF, SVM, BPNN	Accuracy: 100 % (training set) and 99.92 % (test set)	(Ji et al. (2025)
Durum Wheat	255	FT-NIR, FT-MIR	FT-NIR: 10,000-4000 cm^{-1} FT-MIR: 4000-400 cm^{-1}	Determination of OTA content in unprocessed wheat samples	BC, SNV	PCA, PLSR-DA, PC-LDA	Accuracy: 94% (cut-off limit set of 2 μg·kg^{-1} OTA)	(De Girolamo et al., 2019)

ABC: AdaBoost classifier: ABR: AdaBoost regressor; ANN: Artificial Neural Networks; ATR: Attenuated total reflection; BC: baseline correction; BPNN: back propagation neural network; CV: computer vision; DA: discriminant analysis; DON: deoxynivalenol; DT: detrending; EMSC: normalization by extended multivariate signal correction; ETC: extra trees classifier; ETR: extra trees regressor FD: Fusarium damage; FHB: fusarium head blight; FTIR: fourier-transform infrared spectroscopy; K-NN: Naïve Bayes, K-Nearest Neighbours; LDA: linear discriminant analysis; MLR: multiple linear regression; ND: not determined; NIR: near infrared spectroscopy; NIR-HSI: near infrared spectroscopy-hyperspectral imaging; MIR: mid infrared spectroscopy; OTA: ochratoxin A; PCA: principal component analysis; PC-LDA: principal component analysis-linear discriminant analysis; PLSR: partial least squares regression; PLSR-DA: partial least squares-discriminant analysis; RF: random forest; RFC: random forest classifier; RFR: random forest regressor; SAE: sparse autoencoder network; SC: Standard scaling; SGS: Savitzky-Golay smoothing; SROI: selection of spectral region of interest; SVM: support vector machine; SWIR: short-wave infrared; Vis-NIR: visible near-infrared; VN: vector normalization; XGB: extreme gradient boosting; ZEA: zearalenone.

classification models (KNN, RF, and SVM) yielded perfect discrimination between contaminated and uncontaminated samples. These results confirm the viability of using this technology for the rapid assessment of cross-contamination with gluten.

On the other hand, it is important to point out that fungal contamination of food, particularly in cereals, causes significant economic losses. Therefore, it is essential to develop quick, reliable, and economic methods for detecting fungal damage (Hossain & Goto, 2014). A wide variety of spectroscopic methods have been used for mycotoxin analysis including NIR and MIR spectroscopy. These promising tools can be successfully applied to identifying fungal contamination and estimating specific mycotoxins (Freitag et al., 2022). One of the most severe and common diseases of wheat is *Fusarium* head blight (FHB), which is caused by pathogens such as *F. graminearum* and *F. culmorum*. These fungi produce mycotoxins, including deoxynivalenol (DON), zearalenone (ZEA), nivalenol (NIV) and moniliformin (MON), all of which are toxic to animals (Osborne & Stein, 2007). In recent years, numerous studies have emerged evaluating the use of spectroscopic methods to detect fungal infections caused by *Fusarium* in wheat grains and flour (Fig. 4).

For this objective, Almoujahed et al. (2024)explored the ability of NIR and MIR to predict FHB infection of wheat kernels and flour. The contamination range was established by qPCR, covering 0.1–43 ppm of *Fusarium graminearum* biomass. RF and LDA were the two machine learning models used to analyze the collected spectral data. The detection of infected showed higher accuracy for flour samples compared to kernel samples for both spectroscopic techniques, with MIR-LDA reaching 100% accuracy in wheat flour and up to 93% accuracy in whole grains. The classification performance in both regions was comparable for wheat flour samples; however, it was superior in the vis-NIR region for grain samples. Furthermore, Liang et al. (2020) compared the DON levels, classifying wheat samples into normal (<1000 ppb DON) and toxic (>1000 ppb DON), in FHB detection in wheat kernels and flour by different techniques: Vis-NIR and short-wave infrared (SWIR) hyperspectral imaging. In the Vis-NIR range, the results of models obtained with kernel samples were better than those obtained with flour samples, while in the SWIR nm range, the model results showed higher prediction accuracy for flour samples. Similarly, Almoujahed et al. (2025) applied vis-NIR spectroscopy with tree-based machine learning models for DON quantification and classification in wheat grains and flour. The Extra Trees Regressor showed the best predictive performance across the concentration range of 0–49.3 mg/kg. For classification, wheat samples were divided into three categories according to LC-MS reference values: Class 1 (<1.25 mg/kg, suitable for human consumption), Class 2 (1.25–8.00 mg/kg, suitable for feed), and Class 3 (>8.00 mg/kg, destined for bioethanol production). The Extra Trees Classifier achieved the highest accuracy in flour (89.5% accuracy, F1 = 0.89), whereas Random Forest provided the best results in grain (78.9% accuracy).

In this context, NIR spectroscopy has been the most studied technique in recent years for detecting and quantifying mycotoxin content produced by *Fusarium spp.* in wheat flour and grains (Ba et al., 2023; Femenias et al., 2022; Nadimi et al., 2021; Ning et al., 2022; Tyska et al., 2021; T. Zhao et al., 2020). This technology emerges as a useful, rapid, non-destructive, and cost-effective tool that could be valuable for quality control and distinguishing FHB infection in wheat kernel and flour samples during post-harvest stages. Nevertheless, Fomina et al. (2024) also found promising results in the assessment of ATR-FTIR combined with machine learning algorithms for detecting DON contamination in wheat. The prediction models obtained showed high sensitivity and specificity values, as well as high accuracy in cross-validation classification (> 0.840).

Another innovative strategy combines olfactory sensors with spectroscopy to detect mycotoxins such as zearalenone (ZEN), a toxic secondary metabolite produced by *Fusarium* species. Ji et al. (2025) reported that volatile compounds released from infected wheat were captured by a colorimetric sensor composed of six porphyrin derivatives, and the resulting porphyrin spots were subsequently scanned using a portable NIR spectrometer. Among the models tested, the combined PCA–Hippopotamus Optimization (HO)–Random Forest (RF) approach achieved the best performance, with 100% training accuracy and 99.92% prediction accuracy, and was further validated using commercial wheat samples. Importantly, the method successfully discriminated samples with ZEN concentrations as low as 14.03 $\mu g \cdot kg^{-1}$, highlighting its high sensitivity and potential for practical application.

In addition to the mycotoxins produced by *Fusarium spp.*, there are others of considerable importance in cereals, such as ochratoxin A (OTA). Several species of the genera *Aspergillus* and *Penicillium* produce this mycotoxin, which poses a risk to various animal species and humans (Tao et al., 2018). Considering this, De Girolamo et al. (2019) explored the ability of FT-NIR and FT-MIR, in combination with multivariate classification models like PLS-DA and PC-LDA, to discriminate the OTA content in unprocessed wheat samples. For both FT-NIR and FT-MIR, the results showed that the overall discrimination rates exceeded 94% by using a cut-off limit of 2 μg/kg OTA. In conclusion, spectroscopic techniques might be a promising tool to rapidly discriminate fungal

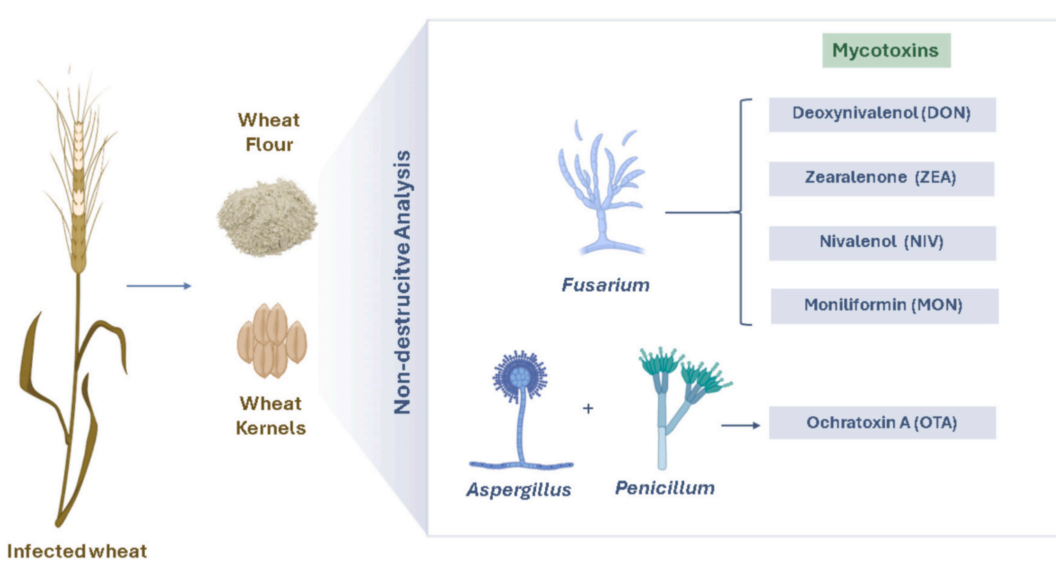

Fig. 4. Detection of fungal contamination in wheat using non-destructive analysis.

contamination in wheat samples

In safety-related applications, contaminants are often present at low and heterogeneously distributed levels, which complicates model development. Reported performance may therefore be optimistic, particularly when based on limited datasets and internal validation without assessment of model transferability.

5. Future Prospects

Despite the extensive research conducted on NIR and MIR spectroscopy for the analysis of wheat flour and wheat-based products, several challenges remain that should be addressed in future studies. While high predictive performance is frequently reported, many calibration models are developed under controlled conditions using limited sample sets, which may restrict their robustness and applicability to real industrial scenarios. Expanding datasets to better capture variability related to cultivar, geographical origin, harvest year, and processing conditions is therefore essential.

The growing use of machine learning and deep learning approaches has further improved predictive accuracy in spectral analysis. However, the application of complex models also increases the risk of overfitting and often relies on internal validation strategies. Future work should place greater emphasis on external validation, model transferability across instruments and environments, and the interpretability of advanced algorithms to ensure reliable and reproducible results.

From a practical perspective, the implementation of NIR and MIR spectroscopy in industrial environments still faces challenges related to calibration maintenance, instrument drift, and sample heterogeneity. Although portable NIR devices and real-time monitoring systems show considerable potential, their long-term stability and robustness under industrial conditions require further investigation. In addition, broader regulatory acceptance and standardized validation protocols will be necessary to support the routine use of spectroscopic techniques in official quality control.

Overall, addressing these limitations will be key to consolidating NIR and MIR spectroscopy as robust, reliable, and widely applicable tools for quality and safety assessment of wheat flour and wheat-based products.

6. Conclusions

NIR and MIR spectroscopy have consolidated their role as rapid, non-destructive, and sustainable alternatives to conventional analytical methods for evaluating the quality and safety of wheat grains and flour. When integrated with chemometrics and machine learning, these techniques have provided robust predictive and categorical classification models addressing both compositional and technological parameters.

Across the reviewed literature, PLSR has been the most widely applied for quantitative prediction, often enhanced by spectral pre-processing and variable selection strategies. For categorical classification, PLS-DA and LDA are frequently employed, while more advanced approaches such as SVM, RF, ANN and GPR have also been successfully implemented to improve model accuracy.

Reliable predictive models have been reported for protein content, moisture, ash, starch, gluten fractions, and mineral composition, with R^2 values frequently above 0.9 and RMSEP values comparable to reference methods. In terms of technological properties, strong predictive performance has been achieved for water absorption, dough strength (alveograph W), and selected GlutoPeak parameters, although other traits such as dough development time, stability, and baking volume remain challenging. Beyond these traits, NIR and MIR spectroscopy have also shown potential in detecting adulteration, verifying authenticity, and monitoring contaminants and allergens, in some cases at levels aligned with or below regulatory thresholds.

Besides, significant research efforts are being devoted to developing miniaturized NIR devices with robustness comparable to benchtop spectrophotometers, aiming to achieve reliable, real-time, on-site analysis.

Overall, the integration of NIR and MIR spectroscopy with both classical chemometric tools and advanced machine learning algorithms provides powerful solutions for quality and safety assessment of wheat grains and flour. Their adoption in industrial practice may reduce analytical costs, enable real-time monitoring, and support sustainable production systems. However, future challenges remain in improving model transferability across cultivars and environments, increasing sensitivity for food safety applications, enhancing the prediction of complex technological traits, and implementing these methods in real-time industrial contexts. Importantly, progress in this field will also depend on the development of standardized and internationally validated protocols to ensure regulatory acceptance and broader industrial application.

CRediT authorship contribution statement

M. Pilar España-Fariñas: Writing – original draft, Conceptualization. **Patricia Cazón:** Writing – review & editing, Supervision, Conceptualization. **María Ángeles Romero-Rodríguez:** Writing – review & editing, Supervision, Project administration, Funding acquisition, Conceptualization.

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Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Data availability

No data was used for the research described in the article.

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