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Predicting loaf volume of white bread by near infrared spectroscopy on wheat flour. Comparative application: NIR reflection, NIR transmission and portable NIR reflection☆

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ABSTRACT

White bread is a worldwide consumed food product with significant nutritional value. The loaf volume of bread is a crucial parameter that influences its texture, appearance and consumer acceptability. Near Infrared Spectroscopy (NIRS) has shown significant potential in predicting the loaf volume of white bread, providing a faster and potentially more accurate alternative to time consuming traditional methods. This study investigates the effectiveness of NIRS and Near Infrared Transmission (NIT) spectroscopy in predicting loaf volume based on wheat flour measurements using both benchtop instruments and a portable FT-NIR instrument. A set of 154 wheat flour samples, including both winter and spring varieties, was analyzed. The performance of NIRS and NIT models was compared with conventional flour analysis methods such as farinograph, alveograph, and rapid visco analyzer. The regression models based on NIR and NIT data demonstrated higher prediction accuracies comparable to traditional methods while significantly reducing both time and complexity of the analysis. This study underscores the potential of NIRS technology to offer rapid and precise predictions of loaf volume, proving to be a valuable tool for baking producers of all scales. Furthermore, the availability of affordable and portable NIR devices makes this technology accessible for small-scale producers, enabling broader adoption across the baking industry.

1. Introduction

According to the Food and Agriculture Organization of the United Nations (FAO) wheat *Triticum aestivum* L. is the third most-produced cereal grain worldwide, only surpassed by Maize and Rice (Awika, 2011). Wheat flour is one of the major food raw materials in the human diet and it is a primary ingredient in many food products such as bread (Ahmed, Randhawa, & Sajid, 2014). Bread stands among the first processed foods crafted by humans and it is prepared by baking fermented dough made from wheat flour, water and yeast (Hidalgo & Brandolini, 2014). The global bread and bakery market continues to grow yearly approx. 6.8 % (CAGR). The growing world population results in an increased demand for food to ensure adequate nutrition for people (Fróna, Szenderák, & Harangi-Rákos, 2019) and analysis of wheat flour for bread making remain a key technology. Determining baking volume is a key aspect of assessing the quality of the flour when baking white bread. This complex parameter is correlated directly with baked products texture, appearance and overall consumer acceptability. Baking volume primarily depends on two factors: the volume of carbon dioxide produced during yeast fermentation, and the gas retention capacity of the dough. These factors are in turn influenced by several underlying parameters: the amount of fermentable simple sugars naturally present in the flour, the starch hydrolyzed into glucose and maltose by amylase enzymes from mixing until baking (when amylase is denatured), and the gluten network developed during dough hydration and mixing. The gluten network, formed by glutenins and gliadins is stabilized primarily through disulfide bridges, provides a visco-elastic structure essential for CO_2 retention. Additionally, physical processes such as dough mixing are critical for developing an effective gluten network capable of entrapping carbon dioxide. Accordingly, an ideal predictive method for baking

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volume should accurately measure flour parameters including simple sugar content, starch content, amylase activity, protein content (especially glutenins and gliadins), and the quantity of disulfide bridges. Accurate measurement and prediction of baking volume thus play a pivotal role in optimizing recipes, ensuring product consistency, and meeting consumer expectations. Measurement of loaf volume through baking test requires skilled personnel, specialized equipment and the associated costs. Therefore, there is a continuous quest for a technique that can predict the baking volume from measurement on the flour. Several methods have been developed, including farinograph and extensograph to predict rheological properties of the dough and loaf volume (Hermannseder, Ahmad, Kügler, & Hitzmann, 2017; Oliver & Allen, 1992). Proposed methods for the prediction of baking performance include a combination of farinograph data with artificial neural networks and stepwise linear regression (Hermannseder et al., 2017) and also within a use of alveograph method (Addo, Coahran, & Pomeranz, 1990; Jodal & Larsen, 2021). In the baking industry, the Mixolab method (Lacko-Bartošová, Konvalina, & Lacko-Bartošová, 2019) is frequently utilized for evaluation the rheological properties and quality of the dough. It measures the force required for mixing flour after addition of water. Mixolab curves gives information about strength of the dough, time development, enzymatic activity as well as pasting properties of the starch (Chung, Ohm, Caley, & Seabourn, 2001; Kahraman et al., 2007; Schmiele, Ferrari Felisberto, Pedrosa Silva Clerici, & Chang, 2017). Loaf volume has also been proposed to be predicted from large deformation rheological properties. Dobraszczyk and Salmanowicz found that the baking volume was predominantly influenced by the strain hardening index, bubble failure strain, and mixograph bandwidth at 10 min (Dobraszczyk & Salmanowicz, 2008). While this technique only needs relatively small sample sizes, it unfortunately requires long run times. As a curiosity it can be mentioned that also seasonal weather data along with neural networks has been used to predict loaf volume (Karki, Glover, Bondalapati, & Krishnan, 2016). Nagael-Held et al. used Fourier-transform Raman spectroscopy (FT-Raman), near-infrared spectroscopy (NIR), fluorescence, and a data fusion approach to predict several parameters in wheat flour, such as protein content, wet gluten, water absorption, plant height, and grain yield. However, in the case of predicting the loaf volume, the authors obtained models with high prediction errors (Nagel-Held, Kaiser, Longin, & Hitzmann, 2022). In this study, the authors did not include RVA, falling number, amylograph, or farinograph parameters in their analysis. In contrast, present study includes a more comprehensive analysis incorporating flour, dough, and baking volume measurements, allowing for a more robust modeling approach.

In this manuscript, we compare the usefulness and limitations of applying NIR reflection, NIR transmission, and portable NIR reflection to predict the loaf volume directly from wheat flour measurements. These results are then compared with a series of conventional flour analysis methods in predicting baking volume. The study is performed on a series of standardized wheat flours from a commercial wheat mill. The techniques presented in this paper have several key advantages. They are fast, require no sample preparation, and are environmentally friendly. Unlike traditional methods, they do not use any chemicals, making NIR technology a green and sustainable solution for flour analysis (Czaja & Engelsen, 2025). Additionally, the development of small handheld NIR instruments enabled a cost-effective and reliable alternative to traditional benchtop instruments. These portable systems are more affordable and highly accessible, enabling smaller mills and bakeries to utilize advanced NIR technology in their operations and to monitor key quality parameters of wheat samples without the need for time-consuming and labor-intensive baking trials. However, NIR spectroscopy cannot directly predict parameters like amylase activity, detailed protein specification (glutenins and gliadins), or disulfide bridges due to their low quantities. Despite these limitations, our hypothesis posits that these factors are interdependent- referred to as the cage of covariance (Eskildsen et al., 2021) – thus allowing NIR spectroscopy to predict baking volume with satisfactory accuracy compared to traditional methods.

2. Experimental

2.1. Material

Wheat flour samples for analysis were collected from Lantmannen Cerealia in Malmö and Strängnäs, Sweden. A total of 154 samples were gathered, comprising both winter and spring wheat. To ensure a diverse range of variations, 105 samples of winter wheat and 49 samples of spring wheat were included. For winter wheat, 45 samples were collected in 2018 and 60 in 2019. In the case of spring wheat, 21 samples were collected in 2018 and 28 in 2019. All samples consisted of sifted flours without any additives and were stored at −20 °C before undergoing spectroscopic analysis.

2.2. NIR and NIT measurements

Near infrared spectra of all flour samples were obtained using three different spectrometers: (1) a general purpose benchtop NIR spectrometer in reflectance mode, (2) a portable FT-NIR spectrometer in reflectance mode and (3) a shortwave benchtop spectrometer designed for transmission NIR spectroscopy (NIT).

The general purpose NIR spectrometer (1) was the FOSS DS2500 spectrometer (FOSS Electric A/S, Hillerød, Denmark) equipped with Silica (400–1100 nm) and Indium gallium arsenide (InGaAs) (1100–2500 nm) detectors. Spectra were acquired in the range 400 nm to 2500 nm, with a spectral resolution of 1 nm in reflectance mode. Each spectrum was an average of 32 scans taken at 8 different positions using a rotating sample cup, resulting in an averaged spectrum combining the 256 scans.

The portable FT-NIR spectrometer (2) was the NeoSpectra scanner (Si-Ware Systems, Cairo, Egypt), which operates within a wavelength range of 1350–2500 nm with scan time 10 s and 5 scans. The spectrometer is equipped with a monolithic micro-electro-mechanical system (MEMS) Michelson interferometer.

The shortwave NIR transmission spectrometer was the Infratec spectrometer (FOSS Electric A/S, Hillerød, Denmark) which operates in the wavelength range from 800 to 1100 nm with a digitalization of 1 nm. The NIR transmission spectra were used to predict protein and moisture content using a build-in calibration.

2.3. Reference analysis

Wheat flour samples were analyzed by a range of classical flour analysis methods some of which have previously been used to predict loaf volume (Selga, Johansson, & Andersson, 2024). In the following the flour laboratory references are briefly described.

Protein content is measured by a prediction method based on the NIT spectra which has been calibrated against a Kjeldahl based reference method.

Moisture content is measured by a prediction method based on the NIT spectra which has been calibrated against an oven drying gravimetric method.

Hagberg falling number is typically used by the baking industry to determine the quality of the flour. It represents an indirect measure of the activity of the hydrolytic enzymes (especially α-amylase) in the flour. The falling number of wheat flour for white bread baking is typically around 250–350. A high number means little enzyme activity (Olaerts et al., 2016).

The Farinograph by Brabender measures and records the dough's resistance to mixing, providing information on key parameters such as water absorption (the amount of water needed for standard dough consistency), development time (time to reach maximum resistance), stability (how long the dough maintains its maximum resistance), degree of softening (dough weakening over time), and the Farinograph Quality Number (FQN), which summarizes overall flour quality and typically ranges from 50 to 100 for wheat bread flour (Technical, 2009a).

The Alveograph test evaluates gluten strength by inflating a piece of dough until it bursts. To perform the test, the dough is initially prepared and developed. Next, disks of dough are cut and left to rest. Each disk is then inflated with air, and its resistance to expansion is measured. This test provides valuable insights into predicting dough behavior and baking quality for various applications, such as bread and confectionery. Additionally, flour millers and manufacturers use the Alveograph test for quality control and product development. Typical values for wheat bread are: P (Resistance to deformation): 60–100 mm H_2O, L (Extensibility): 80–120 mm and W (Baking strength): 200–300 $\times 10^{-4}$ (de Beer, 2023).

Wet gluten is extracted from flour using automatic gluten washing apparatus, then centrifuged. The total wet gluten, expressed as a percentage of the sample, and the gluten index, the percentage of wet gluten remaining on the sieve, are measured. Typical values for total wet gluten for wheat flour are 25–35 % of the sample (Technical, 2009b).

An amylograph measures the gelatinization and viscosity properties of starches during heating, providing insights into their behavior in food products. The gelatinization peak refers to the maximum viscosity achieved during the gelatinization process, indicating the point where the starch granules have absorbed the most water and swelled fully. The gelatinization temperature is the range at which starch granules begin to swell and lose their crystalline structure, marking the start of the thickening process (Juliano et al., 2006).

Rapid Visco Analyzer (RVA) assesses the pasting properties of starches and other ingredients, offering quick and detailed analysis of their viscosity profiles including peak viscosity (maximum swelling capacity), breakdown (starch stability under heat and shear), final viscosity (gel strength upon cooling), setback (retrogradation tendency), peak time (rate of gelatinization), and pasting temperature (onset of viscosity increase) (Balet, Guelpa, Fox, & Manley, 2019; Jackson, 2003).

The white bread baking protocol and loaf volume measurements were performed as described in previous study (Selga et al., 2024) .

2.4. Data analysis

Principal component analysis (PCA) (Bro & Smilde, 2014; Wold, Esbensen, & Geladi, 1987) and Partial least squares (PLS) regression (Geladi & Kowalski, 1986; Wold, Martens, & Wold, 1983) was performed using PLS Toolbox 9.0. Before PCA and PLS data were mean centered. In the case of PLS, calibration models were constructed using either 2nd derivative or 2nd derivative + multiplicative scattering correction (MSC) (Pedersen, Martens, Nielsen, & Engelsen, 2016; Rinnan, Berg, & Engelsen, 2009; Sørensen et al., 2021). The obtained spectra and results of reference baking volume analyses were combined to construct regression models. Using random subset cross validation, the root mean square of cross-validation (RMSECV) was calculated to select an optimal number of PLS latent values. The variable selection was supported by applying forward interval Partial Least squares algorithm (iPLS), evaluating different window sizes to identify the most informative spectral regions. (Nørgaard et al., 2000). To ensure a stratified sampling approach, 25 % of the samples from both the winter and spring datasets were randomly selected as validation set, while the remaining samples were used for calibration purposes. Following model validation, paired *t*-tests were conducted on the predicted bread volume values to statistically assess differences in prediction accuracy between the NIR methods and traditional reference methods. All data processing was performed in Matlab (2022b, MathWorks, Natwick, MA, USA) environment.

3. Result and discussion

Winter wheat typically contains a moderate protein content ranging from 10 to 12 % compared to spring wheat with a higher protein concentration of 12–14 %. The spring wheat is often used specifically for producing bread flour or combined with winter wheat to create versatile all-purpose flour (Gibson & Newsham, 2018). In order to cover a bigger range of variability both winter and spring flour were used in this study. Fig. 1 depicts the distribution of falling number, protein content and loaf volume values. Loaf volume and protein content both reveal a bimodal distribution, distinctly marking separate spring and winter groups. This pattern suggests a relation between protein content and loaf volume. In contrast, the falling number parameter displays a distribution ranging from 300 to 480 without a clear separation between spring and winter flour samples.

Apart from the measurements of protein, falling number and loaf volume also water, ash content, wet gluten, farinograph, amylograph and rapid visco analyzer were also conducted for all wheat flour samples. The Pearson correlation coefficient inter-correlation matrix was calculated for the obtained data, and the results are shown as a heat map in Fig. 2. The analysis shows that loaf volume values correlate with protein content, wet gluten, and development time (from Farinograph analysis). There is no observed correlation with falling number (r = 0.03). The falling number only reveals weak correlations with the farinograph gelatinization peak (r = 0.54) and RVA final viscosity (r = 0.52).

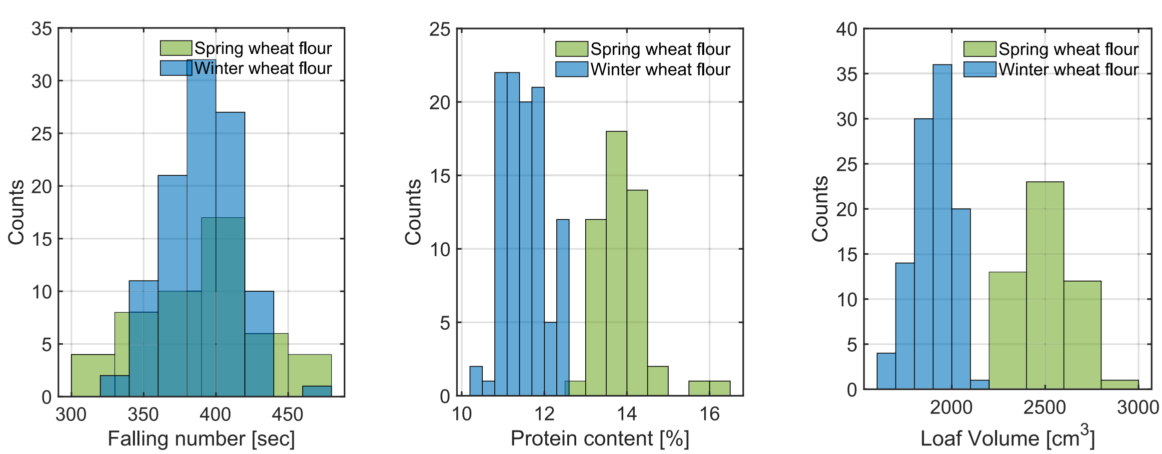

Fig. 1. Distribution of falling number (left), protein content (middle) and loaf bread volume (right) in wheat flour samples. Samples colored according to spring (green) and winter (blue) wheat flour.

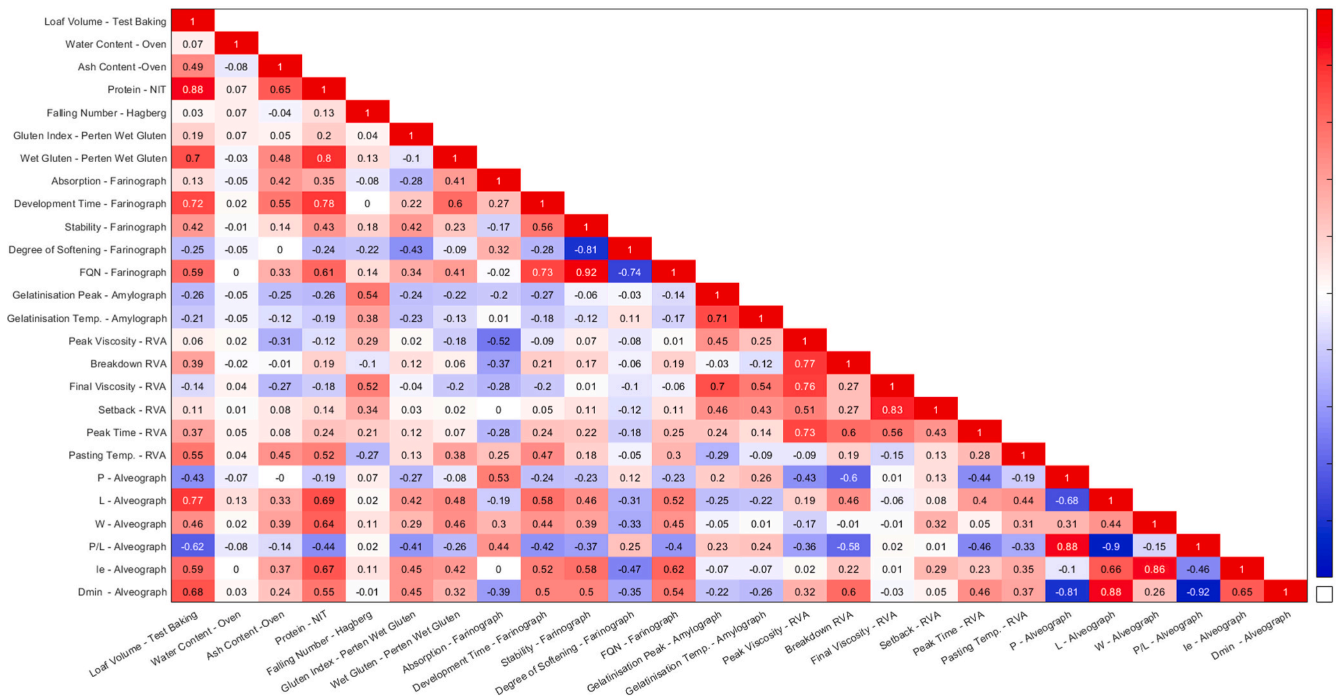

Fig. 2. Heatmap of Pearson correlations among the analyzed flour parameters in the flour lab.

Based on the obtained data, principal component analysis was performed using the auto-scaled data. Fig. 3 shows the PCA biplot of the first two principal components describing 32.06 % and 18.05 %, respectively, of the total variation. The bi-plot shows that the spring or winter wheats are clearly separated along PC1, and equally distributed along PC2. To further illustrate this separation, 95 % confidence ellipses

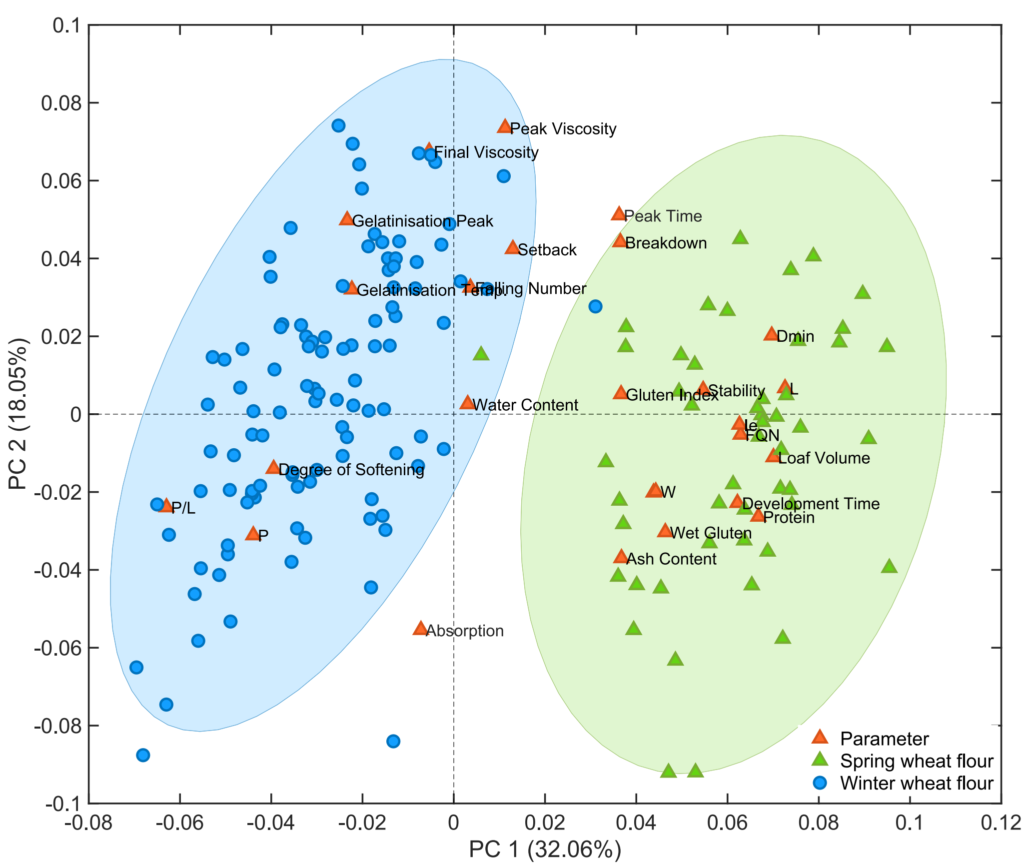

Fig. 3. PCA biplot of 154 flour samples based on reference flour data. Blue circles represent winter wheat flour samples, green circles represent spring wheat flour samples, and orange triangles indicate flour quality parameters (loadings). 95 % confidence ellipses are drawn around each class to illustrate group dispersion.

were added for the spring and winter wheat flour samples. Additional principal components were also analyzed; however, did not yield additional relevant information.

Visual analysis of the biplot shows that the flour quality parameters such as loaf volume, stability and ash are highest in the spring wheat flours, while the degree of softening is highest for the winter wheats. Parameters such as water content, falling number and absorption are located between sample two sample groups, meaning that they are of similar magnitude for the two. The obtained results align with the histograms in Fig. 1, where spring wheat were characterized with higher values of protein content and baking volume, and falling number was distributed across the whole sample set.

3.1. Regression models

The primary aim of this study is to develop a method for predicting white bread loaf volume based on NIR measurements of wheat flour. According to the correlation analysis above the protein content (measured by NIT) is the most promising parameter. However, to investigate this further, we developed baking volume prediction models from: (1) only the protein content parameter, (2) all flour laboratory reference parameters as described in the correlation table and Section 2.3, excluding protein content, (3) NIR reflectance spectra from 400 to 2500 nm, (4) portable FT-NIR instrument 1350–2500 nm and (5) NIR transmission spectra from 800 to 1000 nm.

To develop PLS regression models, the complete set of 154 wheat flour samples was divided into calibration and validation sets. The samples, representing 25 % of each set were randomly selected from both spring and winter flour samples. A total of 117 samples were used for model calibration, while 37 samples were used for validation, maintaining representative distributions of both wheat types in each subset.

Table 1
R^2 and RMSEP of loaf volume prediction based on protein, reference analysis table NIR and NIT.

	Protein content from NIT	Reference analysis table without protein content	Benchtop NIR	Portable FT-NIR	NIT
R^2	0.779	0.838	0.881	0.804	0.848
R^2_{cv}	0.776	0.803	0.863	0.759	0.815
RMSEC	162	118	102	124	116
RMSECV	165	135	116	129	125
RMSEP	161	132	126	138	124
LV	–	3	4	5	3

In the first prediction model (1), only the protein content as determined by NIT, was used for predicting baking volume. The result, shown in Table 1, indicate that this simple univariate regression can predict baking volume with an uncertainty of RMSECV = 162 cm^3 and a squared correlation coefficient of $R^2 = 0.78$. In the second prediction model (2) we use all the quality parameters from the flour lab corresponding to the 24 reference parameters. This model further improved the prediction of the baking volume to an uncertainty of RMSECV = 140 cm^3 and a squared correlation coefficient of $R^2 = 0.81$ (Table 1). The 'measured versus predicted' plots for the loaf volume quantification, based on reference measurements data table and protein content, are gathered in Fig. 4. The next step involved prediction of the baking volume directly from the spectroscopic NIR reflectance and transmission data, allowing for accurate estimation from flour samples without the need for baking. (See Fig. 5.)

The most accurate predictions using NIR transmission spectra were achieved utilizing the 2nd derivative and MSC correction (Pedersen et al., 2016) while for benchtop NIR and portable FT-NIR, only the 2nd derivative was employed. Various preprocessing methods were tested, but these combinations yielded the best results. In all approaches, optimal variable selection was conducted using iPLS to identify the most relevant data segments for loaf volume prediction. The results of the iPLS analysis, including selected intervals, are provided in the supplementary material on Figs. S1-S3. As we have seen above, baking volume is highly correlated with protein. Therefore, for modeling purposes, the combination band (approximately 2290 nm) and the 1st (1960 nm), 2nd (1490 nm), and 3rd (988 nm) overtones of NH bands, which come from protein, were selected. Different wavelength selections were applied for each technique—NIR benchtop, portable FT-NIR, and NIT—though the primary focus on the bands mentioned above. For the spectroscopic models the prediction uncertainties (RMSEPs) was in the same range as the model based on the 24 reference parameters i.e. RMSEP = 126 (NIR), RMSEP = 138 (portable NIR) and RMSEP = 124 (NIT), respectively (Table 1). In case of the R^2 models based on NIR are marginally lowered as compared to the model based on the 24 reference parameters. To further evaluate model performance, residual plots from the PLS regression models are provided in the supplementary material (Figs. S4–S6). Bland–Altman plots based on the calibration datasets for all three spectroscopic models (NIT, NIR, and portable FT-NIR) are also included in the supplementary material (Fig. S7) to illustrate agreement between predicted and reference baking volume values. From the five models it is evident that the lowest prediction accuracies for bread volume are heavily influenced by protein content. It is possible to predict loaf volume directly from the protein content but the error obtained is notably higher than for the other prediction models. The most precise

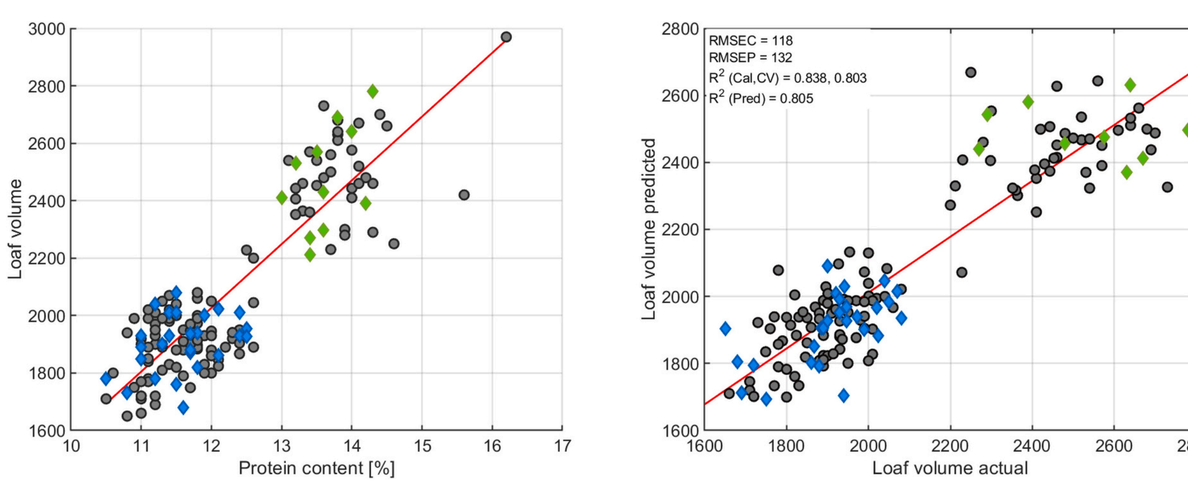

Fig. 4. Prediction plots for loaf volume quantification based on reference measurements data table without protein content (right) and protein content (left). Black circles represent calibration samples. Diamonds indicate validation samples, colored by flour type: blue for winter wheat flour and green for spring wheat flour.

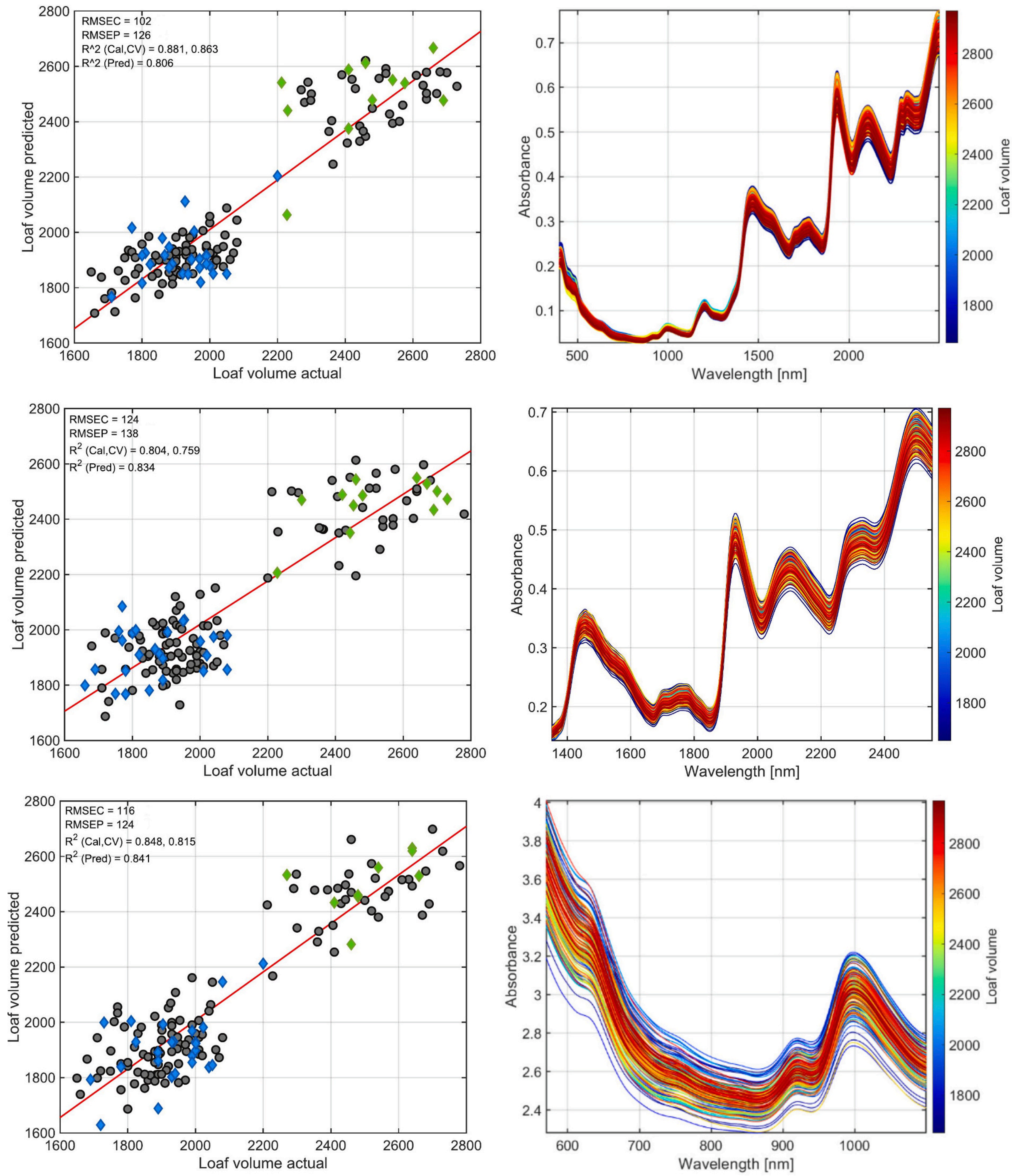

Fig. 5. Prediction plots for loaf volume determination and spectra colored based on loaf volume for, NIR (top), portable FT-NIR (middle) and NIT (bottom). Black circles represent calibration samples. Diamonds indicate validation samples, colored by flour type: blue for winter wheat flour and green for spring wheat flour.

prediction values are obtained using NIR methods, delivering high accuracy with minimal uncertainty in under a minute. Although statistical analysis (paired *t*-tests) showed no significant difference ($p > 0.05$) in prediction accuracy between NIR methods and traditional reference methods for baking volume prediction. NIR offers comparable performance with the added benefits of non-destructiveness and fast analysis. In contrast, reference analysis tables require numerous time-consuming analyses and specialized equipment. Additionally, NIR is a green analytical tool with a negligible CO_2 footprint, making it a superior alternative to traditional baking lab methods.

The results obtained from portable FT-NIR instrument are slightly less accurate compared to NIT and benchtop NIR instruments. However, this opens up the possibility to implement NIR technology in small-scale baking producers and milling companies. This creates an opportunity for smaller businesses to perform rapid and accurate analyses of raw material quality and importantly, predict baking volume directly from flour measurements - without requiring the baking process itself. The development of portable NIR instruments has made them increasingly affordable and more advanced, enabling many small businesses to invest in this technology without relying on laboratory facilities. This provides a cost-effective solution for real-time quality control and analysis directly at production sites. NIR technology is highly versatile and can be calibrated to measure other critical parameters like protein, moisture, starch, and gluten, making it an invaluable tool. With just a single measurement, it's possible to gain insights into multiple factors, such as baking volume, moisture content, and ash levels. This allows small producers to monitor raw material quality easily and ensure consistent, optimized production.

Importantly, NIR technology supports green and sustainable measurement practices. It is ultrafast, requires no chemicals, produces no waste, and is energy-efficient (Czaja & Engelsen, 2025). By using this environmentally friendly solution, producers can improve operations, reduce waste, and contribute to sustainability while minimizing the environmental impact of food production.

4. Conclusion

This study confirms the raison d'etre of NIRS technology in commercial mills and the baking industries. Green NIRS technology provides rapid predictions not only of protein, moisture content, but it is also able to predict loaf volume on par or better to any other quality parameters in the flour laboratory. Even the performance of an easy to use handheld FT-NIR spectrometer gives very good prediction of loaf volume making the method feasible in smaller mills. The techniques presented here eliminate the need for specialized equipment and time-consuming measurements. In combination with chemometrics make also possibilities to measure and determine other parameters in wheat flour. As the demand for sustainable and efficient food production grows, the integration of benchtop and portable, green NIRS technologies provides a forward-looking solution for quality assurance in both large-scale and artisanal milling and baking operations.

CRediT authorship contribution statement

Tomasz Pawel Czaja: Writing – original draft, Formal analysis, Visualization, Data curation, Investigation, Conceptualization. **Louise Selga:** Writing – review & editing, Data curation, Methodology, Investigation. **Roger Andersson:** Writing – review & editing, Investigation, Conceptualization. **Søren Balling Engelsen:** Writing – review & editing, Supervision, 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.

Appendix A. Supplementary data

Supplementary data to this article can be found online at https://doi.org/10.1016/j.foodres.2025.116966.

Data availability

Data will be made available on request.

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