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NYÁRI LADISLAV

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SZÉCHENYI ISTVÁN UNIVERSITY
ALBERT KÁZMÉR FACULTY OF MOSONMAGYARÓVÁR
DEPARTMENT OF BIOSYSTEMS AND PRECISION TECHNOLOGIES

WITTMANN ANTAL MULTIDISCIPLINARY DOCTORAL SCHOOL OF PLANT, ANIMAL AND FOOD SCIENCES

HABERLANDT GOTTLIEB DOCTORAL PROGRAM IN PLANT SCIENCES

Head of the doctoral school:

Prof. Dr. László Varga, DSc

Professor, Doctor of the Hungarian Academy of Sciences

Head of the Doctoral Program:

Prof. Gyula Pinke, DSc Professor

SUPERVISORS:

Prof. Attila József Kovács, DSc Professor

And Dr. Gergely Teschner, PhD Associate Professor

Title of the research topic:

TRACEABILITY OF CEREAL GRAINS AND INVESTIGATION OF THEIR QUALITY PARAMETERS DURING POST-HARVEST OPERATIONS

PREPARED BY:

LADISLAV NYÁRI

MOSONMAGYARÓVÁR

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1. Introduction and Objectives

In the food industry – particularly in cereal processing – traceability is a fundamental requirement from the perspectives of quality assurance and food safety. The increasingly strict regulations of the European Union, together with the need to strengthen consumer confidence, require that the pathway of cereals from the field to the processing plant be documented and verifiable. One of the most critical challenges in practical implementation is the mixing of grain batches during storage and logistical operations, which significantly complicates the accurate identification of origin.

The objective of my doctoral research was to develop a complex traceability system applicable to cereals as granular materials, ensuring the clear identification and traceability of batches throughout the post-harvest chain, including harvesting, cleaning, drying, and storage operations.

The main site of the investigations was AGROSID a.s. – SANAGRO GROUP, a company engaged in grain procurement, storage, and marketing.

The research builds upon my MSc thesis entitled *"Traceability of malting barley production"*, in which I first addressed in detail the practical aspects of traceability in cereal production systems.

The research focused on optical methods, primarily colorimetric analysis based on the CIELAB system and spectrophotometric measurement techniques. Using a reflectance colorimeter equipped with a D65 light source, it became possible to determine the proportion of mixing between different cereal varieties and to quantify the extent of color changes. Based on the measured data, linear trend lines and calibration curves were established, effectively describing the relationship between mixing ratios and changes in color parameters. The application of the HUE × C* index enabled the quantitative evaluation of these changes, providing a precise and objective basis for batch delimitation.

One of the key findings of the research is that mixing ratios can be measured objectively, while color changes characterize the samples in a reproducible manner. This allows the accurate delimitation of grain batches stored in flat storage facilities, the early detection of quality deterioration processes such as *Fusarium* infection, and the reliable traceability of products back to the producer in the event of quality issues.

The integration of optical-based traceability methods into the NOC logistics system represents a new level in cereal storage and processing technologies. The developed system possesses significant scientific and practical value, contributing to the advancement of food safety standards, supporting compliance with European Union regulations, and offering direct applicability in industrial practice.

2. Materials and Methods

2.1. Experimental site

The experiments were conducted between 2021 and 2023 in the southwestern part of Slovakia, on flat lowland areas belonging to the Little Hungarian Plain (Kisalföld), which are characterized by saline soils and an annual precipitation of approximately 500–650 mm.

The experimental region is part of the Great Hungarian Plain (Pannonian Basin) and is located at the northernmost margin of the Danube-associated saline soil complex. The area is characterized by extensive and intensive arable farming, where winter wheat, maize, oilseed rape, sunflower, and other crops are commonly cultivated.

During the investigated years, the total precipitation measured at the experimental plots was approximately 535 mm in 2021, 472 mm in 2022, and 744 mm in 2023.

All experimental plots were located on saline soils, where winter wheat varieties with different grain colors were shown in 2021, 2022, and 2023.

2.2. Experimental material (wheat varieties)

Four winter wheat varieties with distinct grain colors were included in the study: the anthocyanin-rich, purple-grained varieties IS-18W1161 and Karkulka; the yellow-grained variety Bonavita; and the light-brown-grained, conventional variety Genius, which served as the control.

The abbreviations of the investigated wheat varieties and their respective study years were as follows:

- GENIUS (K): light brown grain color; 2021, 2022, and 2023

- KARKULKA (MK): anthocyanin-rich grain color; 2021 and 2023
- BONAVITA I (MB): yellow grain color; 2022
- IS-18W1161 (AG): anthocyanin-rich grain color; 2021, 2022, and 2023
- BONAVITA II (CS): yellow grain color; 2021, 2022, and 2023

Note: The Bonavita variety was grown at two different locations in 2022; therefore, two different abbreviations (MB and CS) were used.

The seed coats of the anthocyanin-rich varieties contain high concentrations of anthocyanin pigments, resulting in an intense bluish-purple grain color. In contrast, the conventional variety accumulates only minimal amounts of anthocyanins, resulting in a typical brownish grain color.

The experimental varieties were cultivated on four different farms within the same region, with each variety shown on a separate agricultural plot. After harvest, the approximately 2.5-ton batches were stored side by side but kept strictly separated. This ensured the availability of clearly distinguishable (color-contrasting) wheat batches for the mixing experiments.

2.3. Sampling and sample preparation

Controlled mixture samples were prepared from the four differently colored wheat batches for the colorimetric experiments. Mixtures were produced for all possible pairwise combinations of the varieties.

In 2021 and 2022, all possible pairwise combinations of the four varieties were investigated (six pairs per year), while in 2023, five variety combinations were examined due to the absence of one pairing.

For each variety combination, mixing ratios were defined between 0% and 100% in 10% increments. Typically, eleven mixing ratios were analyzed for each variety pair, including the pure samples of both varieties. Overall, approximately 60 different mixture compositions were analyzed per year.

Prior to mixture preparation, samples taken from the original batches were cleaned under laboratory conditions. For each variety, 100 g of grain was weighed using an analytical balance and cleaned using a sieve shaker to remove debris and foreign materials.

Calibrated grain sieves (a round-hole sieve with a 1.0 mm aperture and a slotted sieve with a 3.5 mm elongated aperture) and a laboratory sieve shaker (SWING 160) were used for cleaning. Sieving was performed for 5 minutes at a frequency of 140 oscillations per minute. During the process, particles smaller than 1.0 mm (fine dust and debris) and oversized foreign grains and broken kernels retained above the 3.5 mm sieve were removed.

After sieving, only intact and clean wheat kernels (fraction >2.0 mm) were used for preparing the mixtures, ensuring homogeneous sample quality. The desired two component mixtures were prepared by precise mass-based mixing of the cleaned samples.

2.4. Color measurement

From each prepared mixture sample, 200 wheat kernels were selected for color measurement and placed in a single layer into a dedicated sample holder within the instrument’s measurement chamber. This sample size ensured adequate representation of the color characteristics of each mixture.

Color measurements were performed under laboratory conditions using a HunterLab ColorFlex reflectance colorimeter with a 45° illumination and 0° observation geometry. Prior to each measurement series, the instrument was calibrated using standard white and black reference tiles.

Color characteristics were recorded using the standard CIELAB color space, measuring the L* (lightness), a* (red–green), and b* (blue–yellow) parameters for each sample. From these values, the total color difference (ΔE*), hue angle (HUE), and chroma (C*) were calculated and used in subsequent analyses.

Each mixture sample was measured ten times by repeatedly refilling the same 200 wheat kernels into the sample holder, resulting in ten recorded measurements per sample. The mean of the ten measurements was used for evaluation, thereby reducing random measurement error and increasing the reliability of the color data.

2.5. Statistical analysis

A two-step analytical approach was applied to (1) select the most appropriate color variable from nine candidate color variables and (2) evaluate whether homogeneous and heterogeneous parts of grain mixtures of two different wheat varieties could be distinguished based solely on the color variable selected in step one.

In the first step, correlation analysis was performed. The absolute values of Pearson's correlation coefficients (Pearson, 1895) were calculated between the nine candidate color variables and the proportion of the two wheat varieties in 17 grain mixtures. For each candidate color variable, the mean, maximum, and standard deviation of the 17 correlation coefficients were computed. Based on the results (discussed in detail in the subsequent section), the HUE × C* color variable clearly outperformed the others, exhibiting the highest mean and maximum correlation coefficients and the lowest standard deviation. Consequently, the HUE × C* variable was selected for the second step.

In the second step, a linear model was calibrated for each of the 17 grain mixtures, with HUE × C* used as the explanatory variable and the proportion of the two wheat varieties as the response variable. The calibration dataset was used to train the model, which was then applied to predict the variety proportions in the evaluation dataset based on the measured HUE × C* values. Model performance was assessed using multiple metrics, including the coefficient of determination (R^2), adjusted coefficient of determination, and root mean square error (RMSE), calculated for both the calibration and evaluation datasets. In addition, observed and predicted variety proportions were binarized (classified as homogeneous or heterogeneous), and further performance metrics —true positive rate (TPR) and precision—were derived from the model's confusion matrix.

Statistical analyses and data visualization were performed using the R statistical software environment (R Core Team, 2024) and the packages 'caret' (Kuhn, 2008) and 'ggplot2' (Wickham, 2016).

3. Results

3.1. Calibration curves and application of the HUE × C index for modelling the mixing ratios of wheat varieties*

The objective of the doctoral research was to develop and validate a spectral-based methodology suitable for the objective and quantitative determination of mixing ratios of different wheat varieties under storage conditions. The analysis focused on the HUE × C* index derived from spectrophotometric measurements, which proved to be appropriate for modelling mixing ratios.

During the experiments conducted in 2021, pairs of wheat varieties were mixed at different proportions (10–90%), and the resulting spectral data were analysed using statistical methods. The HUE × C* index showed a strong linear relationship with the mixing ratios ($R^2 > 0.90$), allowing the establishment of reliable calibration functions.

These calibration series were repeated in the following years, 2022 and 2023, using grain samples from different harvest years. In 2022, the Karkulka variety was replaced by Bonavita due to limited availability; nevertheless, the results confirmed the reproducibility and applicability of the method. The linear nature of the trend lines demonstrated that increasing or decreasing the mixing ratio resulted in a steady and proportional change in hue.

In 2023, measurements were performed on five mixture combinations, selected due to limited storage availability. The obtained spectral data and the parameters of the trend lines (slope, intercept, and R^2) confirmed the color differences between mixtures and the reliability of the measurement system. The high R^2 values indicate that the data measured by the spectrophotometer accurately represent the color composition of the mixtures. The method enables the precise identification of mixing ratios of wheat varieties stored in warehouses, supports color-based batch delimitation, and enhances traceability. In addition to its scientific relevance, the developed methodology is suitable for practical application, particularly in food logistics and quality control.

It is important to emphasize that the results obtained cannot be directly transferred from year to year. The color parameters of individual varieties varied considerably between harvest years. Consequently, the validity of the model equations is strictly limited to a given year, and separate calibration must be performed for each mixture pair in every experimental year. Although this requirement complicates practical application, it represents an essential scientific finding, highlighting the year-specific influence of environmental and technological factors on color parameters.

3.2. Investigation of storage mixing zones using a spectrophotometric method based on experimental years 2021–2023

The aim of this part of the research was to evaluate how accurately the mixing ratios of different wheat varieties can be quantified under storage conditions using the HUE × C* index derived from spectrophotometric measurements. The analyses were based on previously established calibration curves generated from standard mixture samples.

3.2.1. 2021 – Baseline experiment for the mixing model

In the 2021 experimental year, four wheat varieties with distinct grain colors (K, MK, AG, CS) were poured adjacent to each other, allowing physical contact and the formation of natural mixing zones. Sampling was carried out using a grain sampling probe, starting from the center of the contact zone (zero point) at 30 cm intervals in both directions and across multiple layers. At each sampling point, ten color measurements were performed, and mean values were used for further analyses.

Based on the spectral data, the mixing ratios at each sampling point could be accurately back-calculated using the calibration curves. The HUE × C* index showed a clear and consistent relationship with the mixing ratios of wheat varieties. The reliability of the method was further demonstrated by its ability to determine not only the degree of mixing but also its spatial extent.

3.2.2. 2022 – Evaluation of method reproducibility with different variety composition

In 2022, the Karkulka variety was replaced by Bonavita due to its unavailability. During storage, the AG, MB, CS, and K varieties again came into contact, allowing the observation of grain mixing.

Sampling followed the same protocol as in the previous year, and spectral measurements were again performed with ten repetitions. The results were compared with the graphs obtained from standard mixture samples, confirming that the varietal composition of stored samples could be accurately determined using spectral analysis. The measurements indicated that the effects of mixing could be detected up to approximately 120 cm; beyond this distance, the grain piles could be considered spectrally homogeneous.

3.2.3. 2023 – Confirmation of consistency in calibration and sample analysis

In 2023, similarly to 2021, four wheat varieties with distinct grain colors (K, MK, AG, CS) were poured again using the same arrangement. Sampling and measurement procedures remained unchanged: ten spectral measurements were performed for each sample, and mean values were calculated.

The graphs of standard mixture samples were compared with the measurement results of warehouse samples, allowing the determination of varietal proportions within individual storage batches. Along the spectra of the mixtures (AGCS, MKCS, KCS, MKM, KAG), deviations from the zero axis were clearly documented: the left and right segments of the spectral curves reflected changes in varietal composition. The measurements again confirmed that beyond a distance of 120 cm, mixing was no longer detectable, indicating sharp spectral separation between different wheat piles.

3.3. Application of innovative spectral analysis methods in cereal traceability

During the doctoral research, conventional grain quality assessment methods (moisture content, test weight, protein content, falling number, germination capacity, grading, and DON toxin content) were complemented with spectral analysis.

- The analyses were based on the CIELAB color system, enabling precise and quantitative determination of mixing ratios and color changes.
- Spectral analysis was integrated into the NOC logistics system, allowing objective identification and traceability of grain batches.
- The application of the method ensures:
  - accurate delimitation of stored batches,
  - early detection of quality deterioration processes (e.g., *Fusarium* infection),
  - rapid traceability back to the producer in the event of quality issues,
  - comprehensive documentation from the field to the processing plant.

An important advantage of the system is that data are recorded digitally, eliminating manual errors and enabling long-term trend analysis. Through spectral analysis, cereal quality assessment and traceability have become not only more accurate but also more cost-effective and logistically efficient.

This innovative approach contributes to the advancement of food safety standards and is directly applicable in industrial practice, particularly in the milling and brewing industries, where varietal purity and quality preservation are critical requirements.

4. Conclusions and Recommendations

The aim of our research was to determine how accurately the mixing ratios of different winter wheat varieties can be quantified using spectrophotometric methods. Over the past three years, our investigations generated statistically sound data that enabled the quantitative evaluation of mixing and a detailed description of its spatial distribution. During the spectrophotometric analyses, the parameters of calibration lines were determined, providing a basis for the precise estimation of individual mixing ratios.

Our results clearly demonstrated that the mixing of wheat varieties is not a random process; instead, it depends substantially on the type of the interacting grain batches. For varieties with markedly different grain colors—particularly anthocyanin-rich and yellow-grained wheats—spectral differences were pronounced, allowing clear identification and modelling of mixing zones. This high level of separability enables the application of targeted separation strategies, which can substantially reduce outloading losses and improve quality assurance.

In contrast, when two varieties with similar spectral properties are mixed (e.g., two anthocyanin-rich varieties or two yellow-grained varieties), the differences are minimal and the mixing boundaries become less distinct. In such cases, the methodological sensitivity of color-based spectral analysis approaches its limits, and further analytical refinement is required. An optimal solution may involve the selection of targeted wavelength ranges and the integrated use of complementary optical or chemical methods, which can increase the reliability of delimiting grain batches that appear spectrally homogeneous.

The practical relevance of spectrophotometric investigations extends beyond scientific outcomes. Modelling and spatial localization of mixing processes in storage facilities support the efficient identification of industrial-scale grain batches and, consequently, the optimization of storage and outloading operations. This directly contributes to reducing quality losses and improving logistical efficiency. In addition, the method plays an important role in ensuring traceability within the food chain, which is a fundamental requirement under the strict regulatory environment of the European Union. The application of spectrophotometric analysis enables reliable trace-back of grain batch origin from the field to the consumer, thereby strengthening consumer trust and supporting full compliance with food safety requirements.

In summary, spectral and colorimetric analysis represents an effective tool for investigating the mixing of wheat varieties, particularly when the varieties exhibit distinct spectral characteristics. However, for batches with similar spectral profiles, the sensitivity limits of the method pose challenges that should be addressed through refined analytical strategies and the integration of complementary methods. The results of this research contribute to the development of sustainable and efficient storage strategies, the mitigation of mixing-related losses, and the enhancement of safety and transparency across the food supply chain.

5. Theses

1. **1.** I demonstrated that the C* × HUE color characteristic of the two-component mixtures of the investigated wheat samples can be described by a linear regression model as a function of the mixing ratio. The goodness of fit of the model ranged between R^2 = 0.81–0.98 for the examined mixture pairs, while—excluding varieties with very similar color characteristics—the R^2 values were within the range of 0.90–0.98.
2. **2.** I confirmed that the linear relationship between the C* × HUE color characteristic and the mixing ratio is maintained for the examined mixture pairs regardless of harvest year and mixture composition. Consequently, in practical applications it is sufficient to apply a linear model established from the color characteristics of the pure components, without the need for recalibration.
3. **3.** I demonstrated that, in flat storage environments where mixing zones develop, the C* × HUE-based linear model is suitable for the quantitative estimation of the degree of mixing, as well as for the objective, measurement-based separation of homogeneous and mixed wheat batches.
4. **4.** I established that the applied method is applicable exclusively to two-component wheat mixtures of known composition, and it is not suitable for the comprehensive identification of samples of unknown origin or for full traceability back to the production field.
5. **5.** I demonstrated that the presented methodological approach can be extended to non-contact optical measurement systems (e.g. vision-based systems), and that by incorporating multivariate color descriptors, the sensitivity and robustness of mixing detection can be further enhanced, thereby significantly improving practical applicability.

6. List of Published Works

Peer-reviewed article in an international scientific journal

- Nyári, L. – Dóka, O. – Bede-Fazekas, Á. – Teschner, G. – Baráth, N. – Kovács, A. J. (2026): Cereal storage monitoring using colorimetry: an applied study on grain mixing and zone delimitation in flat storage. Journal of Food and Nutrition Research.

Peer-reviewed scientific articles published in Hungarian-language journals

- Nyári, L., Kovács, A. J., Teschner, G. (2023): Transportation, Storage and Classification of Grain Crops with Consideration of Quality Preservation Aspects. *Acta Agronomica Óváriensis*, Vol. 64, No. 1, pp. 159–193. (35 pages)

- Nyári, L., Dóka, O., Bede Fazekas, Á., Teschner, G., Kovács, A. J. (2026): A Spectral Analysis-Based Methodology for the Storage-Level Separation of Wheat Varieties and the Determination of Their Mixing Ratios. *Acta Agronomica Óváriensis*, Vol. 67, No. 1.

Conference papers published in journals or conference proceedings

- Nyári, L., Kovács, A. J., Teschner, G. (2023): Traceability of Grain Crops during Post-Harvest Operations. In: Molnár, Z., Némethné Wurm, K. (eds.), *Proceedings of the 39th Óvár Scientific Conference*, Mosonmagyaróvár, Hungary, Széchenyi István University, Albert Kázmér Faculty of Mosonmagyaróvár, VEAB Committee of Agricultural Sciences, pp. 29–30. (2 pages)

Conference poster presentation

- Nyári, L., Kovács, A. J., Teschner, G. (2025): Practical Application and Utilization of Grain Traceability during Post-Harvest Operations. Poster presented at the *40th Óvár Scientific Conference*, Mosonmagyaróvár, Hungary. Széchenyi István University, Albert Kázmér Faculty of Mosonmagyaróvár, p. 169.

Article published in a Hungarian professional journal

- Nyári, L., Kovács, A. J. (2026): Post-Harvest Traceability, Handling and Quality Preservation of Grain Crops. *Értékálló Aranykorona*, Hungarian agricultural professional journal.