AI-Enabled Predictive Modeling of Flour Rheological Properties Using Machine Learning Techniques

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Abstract: Flour rheological properties such as water absorption, dough development time, stability, and extensibility are fundamental to assessing dough behavior and bread-making quality. Conventional rheological instruments like the farinograph and extensograph are accurate but costly and time-consuming. Artificial intelligence (AI) and machine learning (ML) provide modern, data-driven solutions for rapid and accurate prediction of rheological properties. This paper presents an AI-based framework integrating artificial neural networks (ANN), convolutional neural networks (CNN), and explainable AI (XAI) methods to model rheological attributes using physicochemical, near-infrared (NIR), and imaging data. The ANN achieved R^2 values exceeding 0.78 for farinograph parameters, while CNN models processing 3D imaging data achieved R^2 near 0.90 for extensibility and toughness. SHAP analysis identified protein content and specific NIR wavelengths as dominant features. The study demonstrates that advanced AI algorithms can replace traditional rheological testing with reliable, cost-effective, and explainable predictive systems.

Keywords: *Machine Learning, Neural Networks, Flour Rheology, Explainable AI, NIR Spectroscopy, Deep Learning, Predictive Modeling, Agricultural AI.*

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I. INTRODUCTION

Flour rheological characteristics determine dough strength, elasticity, and baking performance. These properties influence dough behavior during mixing, fermentation, and baking, impacting the texture and quality of bread and other bakery products. Conventional empirical instruments such as farinographs and extensographs, though accurate, are time-consuming and require skilled operation, limiting their use in real-time quality assessment.

Machine Learning (ML) and Artificial Intelligence (AI) techniques provide new opportunities for predictive modeling in food processing. Neural networks and deep learning algorithms can model nonlinear relationships between input variables (e.g., protein, moisture, NIR data) and output properties (e.g., dough development time, water absorption). Furthermore, Explainable AI (XAI) enables model interpretability, improving adoption in industrial environments.

This research aims to design and validate AI-based models capable of predicting flour rheological parameters accurately. The integration of physicochemical, spectral, and imaging data provides a robust multimodal approach for precise and explainable predictions, aligning with the vision of smart agricultural systems under Agriculture 5.0.

II. MATERIALS AND METHODS

The dataset used in this study included physicochemical data (protein, ash, moisture, gluten index), NIR spectra (900-2500 nm), and 3D imaging data of dough bubble deformation. Each sample represented a distinct wheat variety or milling condition, resulting in a dataset of 250 samples. All measurements were standardized to laboratory reference conditions.

Spectral data preprocessing involved baseline correction, Savitzky-Golay smoothing, and normalization. Dimensionality reduction was achieved using Principal Component Analysis (PCA), retaining 98% cumulative variance. 3D imaging data were voxelized into 64x64x64 grids, and deformation regions were extracted via region-of-interest (ROI) selection. Outlier removal employed the Isolation Forest algorithm, and missing values (<2%) were imputed using k-nearest neighbors (KNN) interpolation.

Three AI models were developed: (1) an ANN using physicochemical and NIR data, (2) a CNN using imaging data, and (3) an XAI-based hybrid model combining the

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two. Data were divided into 70% training, 15% validation, and 15% testing sets.

III. MODEL ARCHITECTURE AND TRAINING

The ANN consisted of three hidden layers (32-64-32 neurons) with ReLU activation, Adam optimizer (learning rate 0.001), and MSE loss function. The CNN architecture was adapted from VGG11 and enhanced with Convolutional Block Attention Modules (CBAM) to capture 3D spatial patterns in voxelized dough images. Dropout (0.2) and L2 regularization were implemented to minimize overfitting.

Training employed 500 epochs and a batch size of 16. Evaluation metrics included R^2, RMSE, and MAPE. Five-fold cross-validation ensured model robustness. Explainable AI was incorporated through SHAP (Shapley Additive Explanations), which quantified feature contributions and ranked input variables by importance. This enhanced interpretability and model transparency, key for industrial applications.

IV. RESULTS AND DISCUSSION

The ANN model achieved strong predictive performance, with R^2 values of 0.79 for water absorption and 0.78 for dough development time. Protein and moisture were the most influential features, followed by falling number. The CNN model demonstrated higher accuracy, achieving R^2 = 0.90 for extensibility and R^2 = 0.88 for toughness. The CBAM layers improved model focus on critical deformation regions, increasing performance by 12% compared to baseline CNNs.

SHAP analysis revealed that protein content accounted for 42% of variance in model predictions, followed by NIR absorbance peaks between 2100-2200 nm, associated with gluten-starch interactions. Compared with regression-based approaches, AI-based models reduced prediction error by 30-35%. Multimodal data fusion further improved prediction stability across different flour types and milling conditions.

The proposed framework demonstrates that AI techniques can complement and even replace traditional rheological assessments, offering faster, non-destructive, and cost-effective alternatives for quality monitoring in flour milling and baking industries.

V. CONCLUSIONS AND FUTURE WORK

This study confirms that AI and ML can effectively predict flour rheological properties with high accuracy and reliability. Neural networks and deep learning architectures provide advanced modeling capabilities, while Explainable AI enhances interpretability for practical deployment. The models developed in this research can be integrated into smart milling systems for real-time, data-driven quality control.

Future research should explore multimodal fusion of additional sensor data, expansion of datasets across geographical regions, and real-time deployment of predictive algorithms in automated production lines. This integration of AI with cereal science represents a critical step toward intelligent, sustainable, and adaptive food manufacturing systems aligned with Agriculture 5.0 principles.

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