

Impact of preharvest conditions and post-harvest processing on quality traits of hard wheat  
(*Triticum aestivum* L.)

by

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B.Tech., Kerala Agricultural University, 2013  
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Department of Grain Science and Industry  
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## Abstract

Hard winter wheat is a key crop in Kansas, primarily used for leavened bread production. The milling and baking quality of this wheat are pivotal for its marketability. Various factors influencing wheat flour's baking quality are: grain variety, agricultural and climatic conditions during growth and harvest, and the milling process. This study investigates the effects of preharvest practices and post-harvest processing on hard winter wheat's baking quality. Specifically, the research aims to: (i) concurrently increase the wheat yield and baking quality through preharvest interventions, (ii) understand the mechanistic aspect of tempering and its impact on wheat kernel behavior, and (iii) assess the role of blending in flour functionality. In the first study, the research investigated the effects of intensive management practices on wheat yield and quality attributes through a factorial experiment conducted across six environments in Kansas. Five wheat genotypes were subjected to four management intensities, including farmer practice, high-input, high-input minus nitrogen, and high-input minus fungicide. Grain yield and 13 parameters representing grain, flour, dough, and baking qualities were evaluated. Results indicated that high -input practices significantly increased yield compared to farmer practice. Application of foliar fungicides improved milling characteristics, while nitrogen-intensive management enhanced the baking quality. Furthermore, improved management positively impacted yield, thousand kernel weight, test weight, grain protein, water absorption, and dough stability. The next stage of research investigated the impact of tempering, a critical step in wheat milling, on wheat kernel properties. A finite element model was developed to analyze moisture distribution within single wheat kernels, finding an effective diffusivity in the range of  $1.63 - 3.81 \times 10^{-11} \text{ m}^2/\text{s}$  for hard red winter (HRW) kernels. The model indicated that the kernel center reached tempering moisture levels in 12h, contrary to the conventional 24h. To enhance predictability, future models could incorporate heterogeneous diffusion characteristics of endosperm, pericarp and germ. Additionally, the study evaluated the influence of tempering on the compressibility of HRW and hard red spring (HRS) kernels through a full factorial experiment. Uniaxial compression tests revealed significant impacts of tempering time on kernel viscoelastic properties. Elastic modulus ranged from 89.2 to 155.8 MPa for HRW and from 115.0 to 192.2 MPa for HRS kernels. Elastic work decreased from 8.8 to 5.4 N.mm, while plastic

work increased to 1.9 N.mm with increasing moisture content. Notably, changes in compressibility followed first order kinetics across all moisture levels, with rate constants ranging from 0.002 to 0.0057 h<sup>-1</sup> for HRW.

Further, the study analyzed the effects of tempering on the chemical and rheological properties of flour from blends composed of different proportions of hard wheat. Blends included B1-25:75 (HRS: HRW), B2-50:50, and B3-75:25. Results indicated significant influence of blending, tempering, and milling streams on protein, damaged starch, and particle characteristics. Protein content varied notably among break flour streams, while damaged starch content varied in the reduction streams across all blends. Higher proportions of HRS led to decreased pasting temperature of the dough. Principal component analysis revealed protein content as a key determinant in flour particle characteristics, water absorption (WA), and pasting properties, especially in blends with higher HRS proportion.

Additionally, an artificial neural network (ANN) model was developed to predict the rheological (farinograph) properties of wheat dough based on flour properties. Multi-layer perceptron type feed-forward ANN models with increasing complexity were developed for each response variable, i.e., ANN-WA, ANN-DDT, and ANN-DS, with optimal models exhibiting the lowest mean squared error (MSE) and highest correlation coefficient (r). ANN- WA and ANN- DDT models demonstrated superior predictive performance when compared to ANN-DS. Feature importance analysis highlighted the significance of flour protein content in the model's prediction. This study demonstrates the potential of data-driven ANN models in predicting the rheological characteristics of dough.

Thus, the comprehensive investigation provides valuable insights into various aspects of hard winter wheat production and processing, aiming to enhance both yield and quality attributes. Furthermore, these findings offer valuable insights into the interplay between tempering conditions and kernel properties, facilitating the optimization of tempering processes for enhanced efficiency. The analysis of flour blends and development of predictive models for dough rheological properties further contribute to our understanding of wheat processing and its impact on product quality.

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## **Dedication**

With deepest gratitude, I dedicate this achievement to my family. Their unwavering love and encouragement fueled me through every challenge and propelled me toward each milestone.

## Chapter 1 - Introduction

Bread has served as a longstanding traditional staple in the diets of millions across centuries (Lockyer & Spiro, 2020). In the United States, annual bread consumption totals 6.64 billion kilograms, equivalent to 19.84 kg per capita, resulting in a substantial revenue of 23.84 billion USD (Wunsch, 2023). Globally, both leavened and unleavened bread products are extensively consumed. The fundamental constituents of bread include cereal flour, water, yeast or other leavening agent, and salt (Gellynck et al., 2009). Notably, among the cereal flours, wheat flour stands out due to its gluten proteins, imparting a unique quality for the formation of elastic dough. Its elasticity, coupled with the capacity to retain gas, renders it a popular choice for leavened products. The baking quality of wheat flour is dependent upon numerous factors, encompassing grain variety, agricultural and climatic conditions during growth and harvest, and the milling process (Collado-Fernández, 2003). For instance, genotype determines characteristics such as kernel hardness, protein composition, and arabinoxylan content (Finnie et al., 2006; Yong et al., 2004). In contrast, factors like grain yield, flour ash, phenolic content and phytochemical are influenced by the environment (Hernández-Espinosa et al., 2018; Rozbicki et al., 2015; Tian et al., 2021). Additionally, crop management practices such as, nitrogen fertilization directly impacts protein content (Giordano et al., 2023; Lollato et al., 2019; Vazquez et al., 2019), which in turn affects the gliadin-glutenin ratio and ultimately, wheat baking quality (Triboi et al., 2000). Therefore, more emphasis is obligatory for preharvest management of wheat as they directly impact the end product quality.

Currently, there is an increased emphasis on technological quality alongside the yield of wheat (*Triticum aestivum* L.). The increased consumption of wheat products underscores the heightened importance of both the nutritional and technological aspects of wheat (Peña-Bautista

et al., 2017). The content and composition of various constituents in wheat play a pivotal role in determining its nutritional and technological quality. As noted by (Johansson et al., 2013), the technological quality of wheat arises from the delicate balance among its numerous components, with significant focus on starch, protein, lipids, and moisture. These constituents are influenced by the genotype, environmental conditions, and cultivation practices (Johansson et al., 2014, 2020). The composition and characteristics of gluten protein, determined by the genotype, contribute significantly to the technological quality of wheat flour, particularly in terms of baking quality.

Increases in grain yield often led to a reduction in grain protein concentration (GP), a phenomenon attributed to GP dilution at higher yields unless accompanied by proportional increases in grain nitrogen (Barneix, 2007; Simmonds, 1995). Recent findings, however, suggest the possibility of concurrently enhancing both yield and GP through effective nitrogen management practices (Lollato et al., 2021). Nevertheless, the end-use quality of wheat depends on various parameters beyond GP, including flour yield, quality, and dough rheological properties (Corassa et al., 2018). Initial investigations into wheat yield and milling and baking quality have predominantly focused on the effects of genotype (G), environment (E) and the  $G \times E$  interaction (Souza et al., 2004; Vázquez et al., 2012; Vazquez et al., 2019; Yong et al., 2004). With limited exceptions (e.g., (Rozbicki et al., 2015; Tian et al., 2022)), the impact of crop management on baking quality has been overlooked. Consequently, the central question remains whether enhancing yield through intensified management practices can also positively influence wheat milling and baking quality parameters.

In addition to pre-harvest conditions, the baking quality of wheat is significantly impacted by post-harvest storage and processing factors. Post-harvest storage conditions, encompassing

temperature, relative humidity, storage duration and moisture content induce alterations in the biochemical composition of the grain and influence baking quality (Hajnal et al., 2014). Within the array of processing conditions influencing baking quality, milling, and blending play pivotal roles. Milling quality is influenced by both wheat kernel properties and operational adjustments of the mills. Kernel properties such as size, size distribution of wheat kernels, density, hardness, and moisture content are critical in determining the flour properties. On the operational side, key factors affecting the milling process include feed rate, roll speed, and roll diameter, roll spiral, roll clearance and type of corrugation, the number of corrugations, roll differential, and grinding pressure (Campbell, 2007; Campbell et al., 2007; Chen et al., 2007; Fang & Campbell, 2003; Sakhare & Inamdar, 2014).

Tempering, a crucial unit operation in the milling process, serves as a pre-conditioning stage involving the addition of a calculated quantity of water to the wheat to achieve a predefined moisture content. After moisture addition, the kernels are stored for a definite period to ensure the migration of water to the kernels. Thus, the process enhances the friability difference between bran and endosperm and helps in the effective separation of the components, bran and endosperm (Cappelli et al., 2020). Typically, hard wheat is tempered to 16 -16.5% moisture content whereas soft wheat is tempered to 14 -14.5%. The tempering process not only affects the energy requirements of milling and particle size (Warechowska et al., 2016) but also exerts an influence on baking quality (Abo-Dief et al., 2019; Kweon et al., 2009).

While the impact of tempering on wheat is well documented, there is a notable gap in understanding the changes that occur within the kernels during the tempering process. Existing studies on moisture migration within the wheat kernels have predominantly focused on soaking, emphasizing time-dependent movement of moisture when kernels are immersed in water.

Surprisingly, there is limited research on the alterations in the migration behavior and compression strength of the wheat kernels specifically during tempering. Comprehensive insights into water uptake, moisture migration and diffusion during the tempering process are provided by studies conducted by (Delwiche, 2000 and Kang & Delwiche, 1999). However, it is noteworthy that these studies primarily limited their modelling endeavors to soaking process. Moreover, the mechanical behavior of food grains is inherently time dependent (Bargale et al., 1995). While numerous researchers have investigated moisture-dependent changes in the mechanical properties of wheat kernels (Escalante-Aburto et al., 2023; Figueroa et al., 2011; Ponce-García et al., 2008, 2013), it is crucial to highlight that in all these investigations, wheat kernels were conditioned for a minimum of 24h at the specified moisture content before conducting experiments. This preconditioning ensured adequate moisture diffusion into the kernel's interior. This highlights the importance of considering the time dependence of moisture distribution when evaluating the mechanical properties of wheat during moisture-related studies. However, current methods often overlook how these mechanical characteristics change throughout the process.

Blending of wheat significantly influences the baking quality of wheat flour by involving the mixing of two or more varieties in specific ratios to achieve desired flour functionality (Alfin, 2019). This process not only ensures consistency in baking quality but also contributes to cost optimization (Hayta & Çakmakli, 2001; Li et al., 2014; Noor et al., 2022). The previous studies on blending predominantly focus on combining wheat varieties within same class or cultivars (Dizlek & Özer, 2017; Levent & Bilgiçli, 2017). The evaluation of blending with varying wheat classes on baking quality of the flour is scarce. Notably, (Simsek, 2020) conducted a study examining the blending of hard red winter (HRW) and hard red spring (HRS) wheat classes to

assess the potential of HRS as a dough improver for clean label whole wheat bread. They demonstrated that an increasing proportion of HRS flour positively influenced the rheological properties (water absorption, and stability) of the dough, along with enhancing the loaf volume of the whole wheat bread. This research highlights a unique perspective on blending across different wheat classes and its impact on dough quality. Moreover, the flour derived from different milling streams exhibits significant variations in biochemical composition and rheological properties. Understanding these compositional variations from blending can influence the functionality of the flour and contribute to process optimization. Understanding how blending different flour affects their functionality is a critical research gap that deserves further investigation.

Rheological properties offer valuable insights into flour quality, encompassing the mechanical behavior of dough during various handling processes (e.g., mixing, dividing, rounding), textural characteristics of the end product, and processing efficiency (Abbasi & Seyedin, 2012).

Commonly employed instruments for measuring these properties include farinograph, extensograph, alveograph, and mixograph (Mutlu et al., 2011). Despite their reliability, these conventional techniques are associated with high costs, time-consuming procedures, and the need for skilled manpower. Consequently, there exists a research gap in the pursuit of developing rapid and dependable methods for assessing the rheological quality of flour, which has the potential to enhance system efficiency. Furthermore, the establishment of models predicting rheological properties using easily measurable flour properties can contribute to online process control in milling industry and modification of process parameters (such as mixing time and speed) in bakeries. Given that the evaluation of high-yield, high-quality varieties by breeding entities often involves expensive milling and baking assessments, such advancements also hold

potential for application in cultivar screening for grain quality within breeding programs.

Consequently, in the final stages of the study, data driven models were employed to predict the rheological properties of the dough. This approach aimed to assess its potential for enhancing the efficiency of quality evaluation.

Thus, the study focuses on addressing the following research gaps:

- Exploring the potential to concurrently enhance wheat yield and baking quality through preharvest interventions.
- Investigating the mechanistic aspects of tempering and comprehending the variations in mechanical behavior of wheat kernels during the tempering process.
- Examining the contribution of blending to flour functionality

As a key ingredient in numerous food products, wheat flour's physical, chemical and rheological properties significantly impact the economic value and final product characteristics. This study's findings can benefit various stakeholders within the wheat supply chain, including farmers, millers and bakers. The study's results particularly those from the first stage can help farmers reduce yield gaps without compromising the baking quality. Understanding moisture migration during tempering can optimize the tempering process, improving efficiency. Additionally, data-driven models could serve as decision support tools, aiding millers in adjusting mill settings based on specific wheat characteristics. The findings on blending studies can be valuable in producing patent flour. Moreover, data- driven models, if further developed, could help bakers modify dough mixing process based on the dough's rheological properties for optimal results.

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## **Chapter 2 – Review of Literature**

Wheat quality is a multifaceted concept with varying importance depending on the stakeholder in the supply chain. For farmers, grain yield is paramount. Millers prioritize test weight and flour yield, while bakers focus on grain protein content and quality. Consumers value the final product – bread loaf quality and nutritional content. One factor uniting all the stake holders is the undesirability of foreign materials in the product.

The thesis aims to investigate the influence of both preharvest conditions and post-harvest operations on the quality of hard wheat. In order to comprehend the impact of preharvest conditions on quality, it is essential to gather information on the composition and morphological characteristics of the kernel, considering how these aspects are affected by environmental conditions and crop management practices. Additionally, post-harvest operations such as tempering and blending, can significantly interfere with the milling and baking characteristics of wheat kernel.

Consequently, a comprehensive literature survey on wheat – encompassing its cultivation, composition and morphological characteristics, as well as the effects of pre-harvest condition and postharvest processing on quality - is imperative. This chapter provides a concise overview of the existing literature that has informed and guided the author in the present study.

### **2.1 Cultivation Status of Wheat**

Wheat (*Triticum aestivum* L.) is one of the oldest cultivated grains, with a domestication history extending back to 10000 years (Uthayakumaran & Wrigley, 2017). In the 19<sup>th</sup> century, different theories emerged regarding domestication of wheat, proposing Near East around Mesopotamia, central Asia and Europe as potential origins (Morrison, 2015; Uthayakumaran & Wrigley, 2017).

Notably, ancient cultivated wheats such as einkorn, emmer, and spelt find their roots in the Fertile Crescent (Arzani & Ashraf, 2017).

Currently, wheat evolved as a crucial staple food source for millions across the globe, supporting nearly 20% of the world's population's caloric and protein needs (Hernández-Espinosa et al., 2018a). Its cultivation spans diverse environments ranging from the equatorial regions to temperate lands (Peña-Bautista et al., 2017). With a global annual harvest exceeding 770 million metric tons, the major wheat producers include China, India, Russian Federation, and USA (FAOSTAT, 2023). *Triticum aestivum*, commonly known as bread wheat, dominates the cultivation, constituting around 95% of the cultivated wheat, while *Triticum durum* or durum wheat accounts for the remainder (Sharma et al., 2020). Wheat's versatility is in its diverse uses, with food consumption comprising the largest significant share at 66%, followed by feed and other industrial purposes (21%) and propagation material (10%) (Erenstein et al., 2022; Psaroudaki, 2007). In terms of average annual per capita food consumption, wheat, at 65.6 kg, holds the second position globally, trailing only behind rice (81 kg). In contrast to rice, which is generally consumed as whole kernels (Siaw et al., 2021) wheat necessitates size reduction before consumption, leading to the production of semolina or flour. In order to optimize flour recovery and guarantee the quality of the final product, it is imperative to understand the composition and morphological features of wheat kernel. Consequently, the following sections provide a brief overview of kernel structure, composition and morphology of wheat.

## **2.2 Wheat kernel**

In the milling of wheat, the primary objective for the miller is to efficiently recover endosperm from wheat bran. The milling quality relies on various factors including the mechanical properties of wheat kernel as well as properties such as mass, shape, size and size distribution of

the kernels (Dziki & Laskowski, 2005). Thus, to maximize flour recovery and ensure the quality of the end product, it is imperative to understand the composition and morphological features of the wheat kernel.

### **2.2.1 Structure**

The wheat kernel is composed of seed and pericarp, with distinct features at its top and bottom ends. At the top, the wheat has fine hairs known as the “brush”, while the bottom region encapsulates the embryo within the germ end (Shewry et al., 2009). The pericarp of the wheat kernel is a complex structure, comprising of multiple layers, including the outer epidermis (15 – 20 µm thick), hypodermis, parenchyma, intermediate cells, cross cells, and tube cells. Collectively, these outer layers are commonly referred to as outer pericarp.

The seed of the wheat encompasses the seed coat (testa), nucellar tissues, endosperm and germ (embryo). The seed coat serves as the outermost layer covering both the starchy endosperm and the embryo. The endosperm, a cellular tissue, contribute significantly to the grain mass, accounting for 80 - 85%. Starch is the predominant component of the endosperm, ranging from 63 to 72%, accompanied by fats and proteins such as gliadins, glutenins, albumin and globulin. The aleurone layer forms the outermost layer of the endosperm.

In milling, the pericarp, testa and aleurone layer are collectively referred to as bran. Bran serves as an excellent source of fiber (53%) and minerals (7.2%), in addition to providing carbohydrates, vitamin B and protein. Approximately, 13 - 17% of the grain mass is attributed to bran, while the germ (embryo) constitutes the remaining 2 - 3%. The embryo consists of the embryonic axis and the scutellum, with the embryonic axis further divided into three regions: shoot (epicotyl), mesocotyl, and radicle. Rich in proteins (25%) including alanine, arginine,

asparagine, glycine, lysine, threonine, lipids (8-13%), vitamin E, and minerals (4-5%), the embryo represents a vital component of the wheat kernel.

A closer examination of the endosperm reveals its composition, characterized by the presence of aleurone layer and the cellular mass enclosed by it. This component serves as the primary storage reserve for starch and protein within the wheat kernel. Starch granules within the endosperm are intricately entrapped in a protein matrix, and the proportion of these cellular components – starch and protein - varies throughout the endosperm (Šramková et al., 2009). Specifically, the proportion of protein increases progressively toward the aleurone layers, while the starch composition increases towards the center (Tosi et al., 2011). The robust interaction between starch and protein is a key determinant of the hardness of wheat kernels, significantly influencing the processing of wheat.

Moreover, the distinctive texture of the endosperm contributes to the floury and vitreous appearance of wheat kernels. Floury endosperm is characterized by the presence of microscopic air cavities, creating a chalky appearance and mechanical weakness for crack propagation. In contrast, vitreous kernels lack these microscopic cavities (Cabas-Lühmann & Manthey, 2020; Shewry et al., 2009). Environmental factors and nitrogen fertilization have been reported to impact vitreousness in bread wheat (Konopka et al., 2015). The genetic control of hardness is another crucial aspect, with a locus on chromosome 5D playing a pivotal role in determining the hardness of both hard and soft wheat varieties. Additionally, the presence of friabilin protein in soft wheat varieties reduces the adherence of starch and protein, consequently reducing hardness (Shewry et al., 2009). This comprehensive understanding shows the interplay of genetic, environmental and compositional factors influencing the structural and processing attributes of wheat.

### **2.2.2 Morphology**

The elucidation of wheat structure hinges on its physical characteristics, encompassing dimensions (length and width), shape, mass, appearance, and color. The length of wheat kernel spans between 4 and 10 mm, with a width ranging from 2 to 5 mm. Several factors, including agronomic conditions, genotype and the grain's position on the spike, contribute to its dimensional variability (Xie et al., 2015). The wheat kernel exhibits an essentially oval shape and is distinguished by a longitudinal crease. Each individual grain, in its dry matter state, weighs between 20 and 60 mg. The surface color of the grain also changes with the factors mentioned above. The surface color of the grain undergoes alterations influenced by the aforementioned factors, typically ranging from golden brown with a reddish hue to a creamy shade.

Moreover, the wheat grain has two discernible sides: the ventral and dorsal sides. The ventral side is characterized by the crease or dissection in the kernel, while the rounded back side constitutes the dorsal side. Notably, the bulk density and true density of the grain vary within the respective ranges of 720 – 830 kg/m<sup>3</sup> and 1200 – 1400 kg/m<sup>3</sup> (Petingco et al., 2020).

### **2.2.3 Mechanical properties**

The mechanical properties of grains play a significant role in milling characteristics, particularly influencing energy consumption during the milling. Research by (Kilborn et al., 1982) indicates a considerable variation in energy requirements, ranging from 42 kJ/kg for soft wheat to 124 kJ/kg for hard wheat. In the milling process, approximately 50% of the power connected with the system is expended to break apart the bran and endosperm and reduce the endosperm to flour. This action leads to heat generation and moisture loss in the ground material. The work of

(Posner & Hibbs, 2005) emphasizes the critical role of wheat kernel texture in determining milling behavior. Understanding these textural characteristics becomes paramount in maximizing milling yield.

The mechanical properties of wheat kernels, associated with the conditions of mechanical separation of the endosperm and the outer bran layer, significantly influence the breaking resistance of the bran, susceptibility of the endosperm and the behavior of starch and proteins during milling (Ponce-García et al., 2013). Commonly these properties are measured through methods assessing the mechanical resistance of kernels to breakage, often evaluated through quasi-static compression studies. Researchers delve into the viscoelastic behavior of kernels, determining their strength and stiffness following standardized procedures like S368.2 and methodologies outlined by Figueora et al., 2008 for measuring individual kernel characteristics. These properties are intricately linked to factors such as kernel moisture content, temperature, rate of loading, as well as the textural characteristics, genotype and growth/ storage conditions. The assessment of these mechanical properties, often conducted through compression tests causing deformations that may or may not be permanent, is crucial for wheat kernels. Fracture strength and hardness, in particular, exhibit a high correlation with yield calculations and milling efficiency (Ponce-García et al., 2017).

### **2.3 Impact of preharvest factors on wheat quality**

The grain's widespread acceptance is attributed to its adaptability across various agro-climatic regions for both growth and storage. Wheat has extensive genetic diversity, with over 25,000 cultivars worldwide exhibiting variations in both physical and compositional grain characteristics (Peña-Bautista et al., 2017). Its broad acceptance is further supported by a high yield potential

and the presence of gluten protein. The viscoelastic properties conferred by gluten enhance the grain's versatility in producing products such as bread, pasta, noodles, cake and cookies (Afzal et al., 2015). Essential determinants of wheat's end use quality include protein content and concentration, starch composition, non-starch polysaccharides and lipids (Johansson et al., 2020).

The rheological behavior of the wheat dough, crucial for product quality, is primarily determined by the protein content comprising gliadin and glutenin. Gliadins, existing as monomeric proteins with  $\alpha$ -,  $\beta$ -,  $\gamma$ -, and  $\omega$ - sub fractions, combine with the polymeric protein glutenin, which consist of low molecular weight (LMW) glutenin and high molecular weight (HMW) subunits. Upon hydration, these proteins form a network in which starch molecules are embedded, providing the foundational structure and rheology of the wheat dough. Factors such as the source of the protein, the molecular weight of the gliadin and glutenin, and the gliadin - glutenin ratio play pivotal roles in influencing the rheology of wheat dough (Shewry et al., 1986). The viscoelasticity of gluten is further influenced by the quantity and composition of high molecular weight glutenin.

The functionality of wheat grains is intricately tied to environmental, genetic and management factors (Filip et al., 2023; Nuttall et al., 2017). The subsequent sections will delve into a detailed exploration of these factors.

### **2.3.1 Environmental factors**

The quality of wheat for end – use applications is significantly influenced by temperature and precipitation patterns during the early stages of grain development and grain, as highlighted by (Hernández-Espinosa et al., 2018b). The optimum temperature for wheat grain filling is reported to be between 20 and 22 °C, as indicated by (Zhao et al., 2022). Extreme temperatures during

growth and grain filling can have adverse effects on both yield and grain composition (Table 2.1). Day time temperatures exceeding 30 °C during grain filling are associated with reported yield decrease ranging from 6 % to 51% (Bergkamp et al., 2018).

Temperature stress not only affects yield but also alters various morphological characteristics of the wheat grain. Width and length of the grain, kernel density, size and 1000 kernel weight are all reduced under temperature stress. The stress modifies the grain filling duration and rate, further impacting morphological features (Hernández-Espinosa et al., 2018b; Zhao et al., 2022). Heat stress during the grain development adversely affects starch biosynthesis, leading to a reduction in starch content and an increase in protein content (Wang et al., 2018). High temperatures can cause the inactivation of enzymes involved in starch synthesis, hindering the conversion of sucrose to starch and resulting in diminished starch content (Lu et al., 2019). (DuPont & Altenbach, 2003), suggest that the reduction in starch content under heat stress is attributed to the premature cessation of starch accumulation, thereby shortening the time to reach maximum grain weight.

Temperature stress impact the composition of starch, with reductions observed in amylose, amylopectin and total starch content (Zhao et al., 2022). Additionally, temperature stress increases the  $\alpha$  – amylase activity, leading to decomposition of starch and modification of starch granule morphology (C. Y. Li et al., 2017). The heat stress – induced changes extend to the protein composition of grain, with an increase in high molecular weight glutenins (HMW-GS) and  $\omega$ - gliadins. This alteration affects glutenin content, the gliadin - glutenin ratio and overall protein concentration in the grain (Zhao et al., 2022).

Limited water availability during growth stages emerges as a critical determinant affecting wheat grain weight, as noted by (Anwaar et al., 2020). Drought stress disrupts starch synthesis

enzymes, diminishing the rate of starch synthesis and subsequently resulting in decreased starch content and grain weight (Lu et al., 2019). Furthermore, drought stress induces an increase in the protein content and polymeric protein of wheat grain, as evidenced by research conducted by (Guttieri et al., 2001). The imposition of water stress conditions triggers a partial closure of stomata, reducing the carbon fixation. Simultaneously, the remobilization of nitrogen from leaves to grains occurs, leading to a decrease in grain weight and an increase in protein percentage (Souza et al., 2004). Additionally, lipid content experiences a reduction under drought stress conditions, as reported by (Silva et al., 2020).

The reduced water availability extends to nutrient uptake by roots, resulting in a decrease in both macro and micronutrients (Bista et al., 2018). Furthermore, the concentration of atmospheric CO<sub>2</sub> during the grain filling emerges as an influential factor, influencing starch and protein deposition and consequently impacting dough rheology (Nuttall et al., 2017). This integrated understanding highlights the intricate interaction among various environmental stressors and their cumulative effects on the morphological and compositional attributes of wheat grains.

### **2.3.2 Genotype**

The morphological characteristics of wheat grains, encompassing shape, dimensions and color, exhibit considerable variation based on type and cultivar of wheat, as observed by (Bechtel et al., 2009). The genetics determinants of grain hardness lie in the presence or absence of puroindolines encoded by specific genes (Johansson et al., 2020). These puroindolines play a pivotal role in influencing the adhesion of storage proteins with starch within the wheat grain.

Protein content and composition are fundamental factors influencing the end use quality of wheat grain. The genotype significantly contributes to determining protein quality, encompassing aspects such as protein composition, the glutenin–gliadin ratio, and the extraction with sodium

dodecyl sulfate (SDS) value, (Hernández-Espinosa et al., 2018b). The intricate relationship between genotype and protein characteristics underscores the genetic influence on the overall quality of wheat grain.

### **2.3.3 Management practices**

The significance of management practices in enhancing wheat grain quality is highlighted in studies by (Torrión & Stougaard, 2017) and (Zecevic et al., 2010). Notably, nitrogen fertilization stands out as a crucial factor influencing various grain characteristics. Nitrogen application has a direct impact on grain protein content, wet gluten content and the gliadin–glutenin ratio (Daaloul Bouacha et al., 2014; Lollato et al., 2019, 2021; Mohammed et al., 2013; Triboni et al., 2000; Vazquez et al., 2019; Zecevic et al., 2010). The timing of nitrogen application has been shown to improve protein content in grains (Corassa et al., 2018; Cruppe et al., 2017; Giordano et al., 2023; Lollato et al., 2021). Nitrogen also exhibits interactions with sulfur fertilization, influencing grain asparagine concentration (Wilson et al., 2020). Some studies additionally report an increase in the concentration of  $\omega$ - gliadins and low molecular weight (LMW) glutenins with increased nitrogen application, with a more pronounced impact on gliadins compared to glutenins (Wieser & Seilmeier, 1998; Zörb et al., 2018). The application of sulfur has been found to increase glutenin content, comprising both low molecular weight glutenins and high molecular weight glutenins, consequently improving the rheological properties of the flour (Cai et al., 2022).

Another critical management practice influencing wheat yield is the use of foliar fungicides, as noted by (Cruppe et al., 2021) and (Sassenrath et al., 2019). The combination of higher nitrogen rates with foliar fungicide has been shown to maintain grain protein content despite improvements in yield (de Oliveira Silva et al., 2020; Fleitas et al., 2018). This effect is

attributed to increased leaf area duration and prolonged nitrogen uptake and translocation ((De Oliveira Silva et al., 2021; Schierenbeck et al., 2019). The integration of management practices provides valuable insights into optimizing wheat grain quality and yield through agricultural interventions.

## **2.4 Impact of postharvest factors on quality**

After harvest, wheat grains undergo post-harvest maturation, a process that extends into storage and is contingent upon storage conditions such as temperature, relative humidity, storage duration and moisture content of the grains. These storage conditions induce changes in the biochemical composition of the grain, ultimately impacting baking quality (Hajnal et al., 2014). (González-Torralba et al., 2013) noted that post-harvest storage of hard wheat modifies the milling and baking quality. Additionally, tempering and blending are identified as other post-harvest operations that can influence the milling and baking quality of wheat. The subsequent sections will delve into the details of tempering and blending, elucidating their specific influences on milling and baking quality.

### **2.4.1 Tempering**

Tempering, a crucial initial stage in the wheat processing, involves addition of water to the kernels, allowing them to rest for a specified duration before milling. This preconditioning process, as outlined by (Posner & Hibbs, 2005), ensures that the kernels attain an optimal moisture distribution, rendering them suitable for the milling process. The overarching objective is to toughen the bran and soften the endosperm, ultimately enhancing the efficiency of flour extraction ((Kweon et al., 2009). Consequently, this stage assumes significant importance from technical, flour quality and economic perspectives within the broader context of wheat

processing. The intricacies of water uptake and moisture migration during tempering are subject to various influencing factors, including temperature, initial moisture content, time and kernel hardness (Delwiche, 2000; Kang & Delwiche, 1999; Posner & Hibbs, 2005). Researchers have extensively explored the impact of tempering moisture content on granulometric properties (Fang & Campbell, 2003) and energy consumption during milling (Warechowska et al., 2016). This broad spectrum of studies underscores the comprehensive analysis of the tempering from both mechanistic and functional perspectives, contributing to an understanding of its role in optimizing milling outcomes and ensuring the production of high-quality flour (Table 2.2).

Advanced milling systems are commonly integrated with computer control systems to manage moisture addition in the tempering system, employing various components such as paddle screw conveyors, intensive dampeners, and turbolizers, as well as regulating the residence time of grains in tempering bins (Alfin, 2020). The understanding of moisture distribution within kernels plays a pivotal role in determining the moisture addition during the tempering process. This knowledge is particularly beneficial for systems like moisture proportioning system (eg., MOZG) and moisture control system. Maintaining a uniform moisture distribution across kernels is essential, enabling the application of high-water additions of up to 7% in a single pass (Kunz, 2016). Furthermore, uneven moisture distribution within kernels may lead to water movement towards the tempering bin outlet, potentially causing blockages. The implementation of mathematical models capable of accurately predicting variations in moisture content around the target moisture content becomes crucial for the effective regulation of processing system.

#### **2.4.1.1 Moisture migration**

Early investigations into the migration of water through wheat kernels were reported by Fritsch (1940), who proposed a theory involving capillary tubes extending into the interior of the

kernels, facilitating the transfer of moisture. Subsequent studies by (Grosh & Milner, 1959) delved into the tracking of moisture movement through cracks in the wheat kernel, revealing the formation of radial and transverse cracks within an hour of wetting the kernels. Building on this, (Moss, 1977) employed titrated water to create an autoradiographic pattern detailing the rate and distribution of water within the kernel. The results indicated that labeled water penetrated the aleurone layer within 1h, while the germ and scutellum rapidly absorbed water. In contrast, penetration to the starchy endosperm experienced a delay of several hours. This investigation highlighted the variability in moisture absorption patterns among different layers of the wheat kernel. Crucially, the diffusion of moisture inside the kernels is contingent upon the diffusion constants.

#### **2.4.1.2 Mathematical models describing moisture migration in wheat kernels**

The general analytical solution for of the moisture addition with respect to time was obtained by integrating the concentrations over the volume of kernel following Fick's diffusion theory. The solution of the diffusion equation (Eq. 2.1) is:

$$MR = \frac{m_t - m_{in}}{m_{eq} - m_{in}} = \sum_{n=1}^{\infty} B_n \exp(-A_n^2 t)$$

MR = moisture ratio (dimensionless quantity ranging from 0 to 1)

$m_t$  = average moisture content at time t (% , dry basis)

$m_{eq}$  = equilibrium moisture content at kernel surface (% , dry basis)

$m_{in}$  = initial moisture content of whole kernel region (% , dry basis)

$A_n$  = constant

$B_n$  = constant for given solid shape

$$F_o = \text{Fourier number} = Dt/L_c^2$$

$$D = \text{Diffusion coefficient (m}^2/\text{s)}$$

$$t = \text{time variable (s)}$$

$$L_c = \text{characteristic length (m)}$$

For a sphere,

$$B_n = \frac{6}{A_n^2}$$

$$A_n = n\pi$$

$$L_c = 3 \times \frac{\text{volume}}{\text{surface area}} = r_s = \text{radius of sphere}$$

For an infinite cylinder,

$$B_n = \frac{4}{A_n^2}$$

$$A_n = r_c \alpha_n = \text{nth positive root of Bessel function } J_0(r_c \alpha_n) = 0$$

$$J_0(x) = \text{Bessel function of the first kind of order zero}$$

$$L_c = 2 \times \frac{\text{volume}}{\text{surface area}} = r_c = \text{radius of cylinder}$$

For an infinite plane sheet,

$$B_n = \frac{2}{A_n^2}$$

$$A_n = (2n - 1)(\pi/2)$$

$$L_c = \frac{\text{volume}}{\text{surface area}} = l_0 = \text{half thickness of sheet}$$

Among analytical solutions for various geometries mentioned earlier, the wheat kernel has the closest resemblance to a sphere. Therefore, the analytical solution for a sphere is widely chosen for studies involving wheat kernel.

Babbitt (1945) conducted mathematical modelling to analyze moisture migration in wheat kernels employing thermodynamic characterization of equilibrium hydration. Assuming the wheat kernel as a homogeneous sphere, vapor diffusion coefficients were calculated. This assumption was widely adopted in subsequent moisture diffusion studies and soaking experiments on wheat kernels. Hinton's (1955) research revealed lower diffusion rates in pericarp compared to the endosperm, necessitating separate determination of diffusion coefficients for each component. In response, (Igathinathane & Chattopadhyay, 1997) developed a finite element model (FEM) for grain soaking considering the wheat kernel as a 'composite sphere having starchy endosperm core and an outer concentric shell of bran'. As a result, the diffusivity of the endosperm was calculated as  $1.91 \times 10^{-10} \text{ m}^2/\text{s}$  and that of bran as  $1.78 \times 10^{-10} \text{ m}^2/\text{s}$ . (Kang & Delwiche, 1999) further modified the models and introduced a non-spherical geometry correction, incorporating circularity and ellipticity for a more accurate prediction of moisture migration. It was concluded that, for an improved estimate of moisture diffusion coefficients, modifying the geometry to a prolate spheroid using sphericity and ellipticity as correction factors is crucial. Consequently, the moisture diffusion coefficient ranged from  $0.39 \times 10^{-10} \text{ m}^2/\text{s}$  to  $1.04 \times 10^{-10} \text{ m}^2/\text{s}$  for endosperm and  $0.04 \times 10^{-10} \text{ m}^2/\text{s}$  to  $0.28 \times 10^{-10} \text{ m}^2/\text{s}$  for the pericarp. The overall consensus is that a numerical solution based on proper geometrical shape is essential for accurately predicting moisture transfer in wheat kernels.

The existing literature primarily focuses on moisture migration within kernel based on soaking them in water, overlooking the modifications that occur in the tempering process where water

availability is limited. While the milling quality implications of tempering have been extensively studied, there is a notable gap in research from an engineering perspective, particularly in understanding its influence on the mechanical properties of the wheat kernel. Therefore, there is a critical need to investigate moisture migration within kernels during the tempering process and comprehensively assess the impact of tempering on the mechanical characteristics of the kernels.

### **2.4.2 Blending**

Blending of wheat or flour is a critical step in the processing of wheat. The process helps to maintain the consistency in the end use quality of the flour for the customers (Issarny et al., 2017). Environmental factors and agricultural practices significantly influence wheat quality, causing variations even within the same variety (Raj et al., 2023; Rozbicki et al., 2015; Tian et al., 2022; Vazquez et al., 2019). This variability necessitates blending, the mixing of different wheat types or varieties to achieve consistent flour quality and manage costs (Alfin, 2019; X. Li et al., 2014). Blending involves combining wheats of varying quality to arrive at desired flour characteristics (Hayta & Çakmakli, 2001). Beyond chemical composition, the chosen wheat varieties can differ in physical properties, impacting flour particle size and ultimately, quality. While existing literature addresses wheat blending, it primarily focuses on blending within the same cultivar. For example, (Dizlek & Özer, 2017) investigated improving damaged wheat functionality through blending with undamaged wheat of the same variety. Similarly, (Levent & Bilgiçli, 2017) studied blends of the same cultivar harvested at different maturities, analyzing the impact of blending ratios on the physicochemical and rheological properties of straight-grade flour.

While there are numerous studies investigating the impact of tempering on flour quality and the biochemical variations in milling streams, research on the effects of blending on the composition

and rheological parameters of flour are limited. A deeper understanding of compositional variations resulting from blending would contribute to the optimization of the hard wheat milling process in terms of both quality and cost. Therefore, further studies on hard wheat blending and its influence on flour functionality are needed.

## **2.5 End use quality**

The end use quality of wheat is influenced by various factors such as protein content, kernel weight, gluten content, milling yield, falling number value and rheological properties (Mutlu et al., 2011). Protein content, a primary determinant of wheat quality in baking, has a significant impact on bread loaf volume and dough rheological properties (Corassa et al., 2018; Koppel & Ingver, 2010; Park et al., 2006). Amylase activity, measured through falling number analysis, is another crucial parameter affecting flour's baking quality and influencing dough development time (Dencic et al., 2013; Hu et al., 2022). Moisture content also plays a role in water absorption, affecting the workable consistency of the dough. The mechanical properties of the kernel contribute to the physicochemical properties of the flour, guiding the selection of wheat cultivars for processing and end-use (Ponce-García et al., 2017).

The study of intact kernels has been utilized to establish relationships among protein composition, viscoelasticity of dough, and baking outcomes (Figueroa et al., 2009, 2012). By investigating the viscoelastic characteristics of glutenins in wheat kernels, (Hernandez-Estrada et al., 2012; Hernández-Estrada et al., 2014; Hernández et al., 2012) developed correlations with SDS sedimentation and rheological properties. Understanding the viscoelastic properties of individual wheat kernels becomes instrumental in determining the extent to which these properties transfer to the dough.

Rheological properties offer valuable insights into flour quality, the mechanical behavior of the dough during handling processes, textural characteristics of the final product, and processing efficiency (Abbasi & Seyedin, 2012). Traditional instruments like farinograph, extensograph, alveograph, and mixograph are conventionally used to measure these properties (Mutlu et al., 2011). However, these methods, while reliable are associated with high costs, time consuming procedures, and the need for skilled technicians.

Artificial neural networks (ANNs) emulate the biological nervous system to map nonlinear relationships between input and output, offering flexibility, robustness and adaptability (Abbasi et al., 2014; Raj & Dash, 2020b). These computational models find application in various domains, including food safety, quality analysis, and modelling thermal and non-thermal operations (Raj & Dash, 2020a). A comprehensive review on the application of ANN in food (Ayed & Hanana, 2021; Raj & Dash, 2020a) provides an extensive overview of the available literature. Over the past decade, several ANN models have been developed to predict the rheological properties of wheat flour (Abbasi et al., 2014; Mutlu et al., 2011; Razmi-Rad et al., 2007). Feed forward multilayer perceptron (MLP) models, developed by (Abbasi et al., 2014) and (Razmi-Rad et al., 2007), predict farinograph quality parameters based on chemically analyzed flour properties (protein content, ash content, wet gluten content, gluten index, Zeleny sedimentation value, and falling number value). (Mutlu et al., 2011) explored the potential of ANN to predict dough quality using near-infrared (NIR) spectra of flour. Although these models have successfully identified parameters for predicting farinograph attributes, their ability to predict outcomes on unfamiliar datasets is constrained by the small dataset size employed during training and testing. Furthermore, the rationale behind the predictions or the decision – making process of the models is often overlooked.

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## Tables

**Table 2.1. Effect of environmental conditions on wheat quality**

| <b>Environmental factors</b> | <b>Quality affected</b>             | <b>Impact</b> | <b>References</b>                          |
|------------------------------|-------------------------------------|---------------|--------------------------------------------|
| High temperature             | Starch                              | Decrease      | (Mariem et al., 2021)                      |
|                              | Grain protein concentration         | Increase      | (Mariem et al., 2021; Sissons et           |
|                              | • High molecular weight glutenin    | Increase      | al., 2018)                                 |
|                              | Lipids                              | Increase      | (Impa et al., 2020)                        |
|                              | Minerals                            |               |                                            |
|                              | • Mg                                | Increase      | (Mariem et al., 2021)                      |
|                              | • Ca, Fe, Mn, Zn                    | Decrease      | (Mariem et al., 2021)                      |
|                              | Thousand grain weight               | Decrease      | (Aiqing et al., 2018; Mariem et al., 2021) |
|                              | Test weight                         | Decrease      | (Sissons et al., 2018)                     |
|                              | Milling yield                       | Decrease      | (Sissons et al., 2018)                     |
| Water stress                 | Starch                              | Decrease      | (Ahmadi & Baker, 2001)                     |
|                              | Grain protein concentration         | Increase      |                                            |
|                              | • High molecular weight glutenin    | Increase      | (Zörb et al., 2017)                        |
|                              | • Gliadin                           | Decrease      |                                            |
|                              | Lipids                              | Decrease      | (Silva et al., 2020)                       |
|                              | Soluble and insoluble bound phenols | Increase      | (Graziano et al., 2019)                    |
|                              | Minerals                            |               |                                            |
|                              | • Fe                                | Increase      | (De Santis et al., 2021)                   |
|                              | Thousand grain weight               | Decrease      | (Anwaar et al., 2020; Zhang et al., 2017)  |
|                              |                                     |               |                                            |

**Table 2.2. Effect of tempering on the end use quality parameters of wheat**

| Tempering condition         | Levels                   | Quality parameters with corresponding increase in tempering conditions                       |                                                                                                                               | References                                          |
|-----------------------------|--------------------------|----------------------------------------------------------------------------------------------|-------------------------------------------------------------------------------------------------------------------------------|-----------------------------------------------------|
|                             |                          | Increases                                                                                    | Decreases                                                                                                                     |                                                     |
| Moisture                    | 12% to 18%               | Sucrose solvent retention capacity (SRC)<br>Lactic acid SRC<br>Stability<br>Water absorption | Milling yield<br>Ash content<br>Protein content<br>Polyphenol oxidase (PPO)<br>Sodium carbonate SRC<br>Dough development time | (Kweon et al., 2009);<br>(Warechowska et al., 2016) |
| pH                          | 3, 4, 5, 6, 7            | -                                                                                            | Milling yield<br>Ash content                                                                                                  | (Yoo et al., 2009)                                  |
| Time                        | 3h to 36h                | Milling yield<br>Moisture content<br>Ash content<br>PPO<br>sodium carbonate SRC              | Protein content<br>Gluten index<br>Sucrose SRC<br>Lactic acid SRC                                                             | (Abo-Dief et al., 2019; Kweon et al., 2009)         |
| Temperature                 | 25 and 45 °C             | Sucrose SRC<br>Lactic acid SRC                                                               | Milling yield<br>Ash content<br>PPO<br>Sodium carbonate SRC                                                                   | (Kweon et al., 2009)                                |
| Steam tempering (0.64 kg/h) | 160, 200, 240, 280, 320s | Ash content<br>Dough development time<br>Stability                                           | Milling yield<br>Particle size                                                                                                | (Chen et al., 2020)                                 |

## Figures

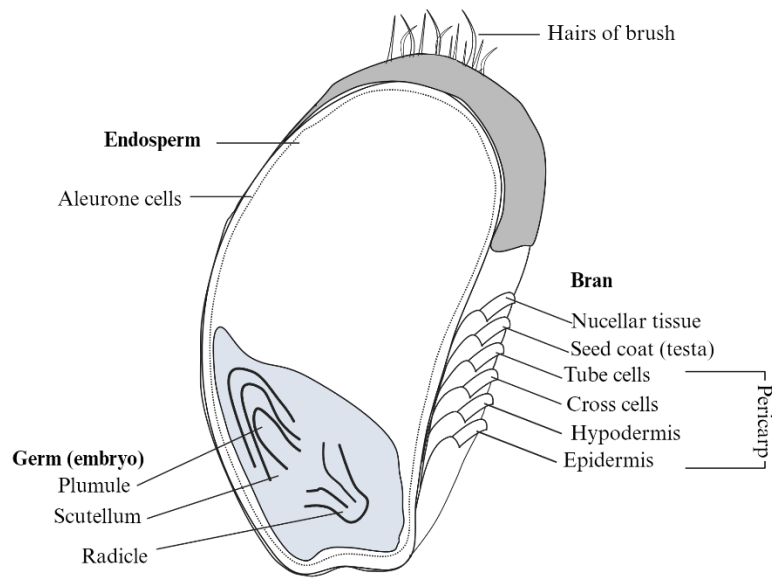


**Figure 2.1. Structure and composition of wheat (Sramkova et al., 2009)**

## **Chapter 3 – Intensive management simultaneously reduces yield gaps and improves milling and baking properties of bread wheat<sup>1</sup>**

### **Abstract**

Genotype (G), environment (E), management (M), and their interactions determine grain yield, biochemical composition, and quality of wheat. However, we are not aware of studies evaluating whether intensive management can simultaneously reduce yield gaps and improve wheat milling and baking attributes, which was our main objective. A factorial experiment of five genotypes by four management intensities (farmer practice, high-input, high-input minus nitrogen, and high-input minus fungicide) was conducted in six Kansas (US) environments resulting from the combination of four locations and three seasons. Grain yield and 13 parameters characterizing the grain [test weight (TW), thousand kernel weight (TKW), grain protein (GP)], flour (e.g., ash, protein), dough [e.g., water absorption (WA), dough stability (DS)], and baking qualities [loaf volume (LV)] were measured. For most variables, the primary contributor of the variance was E while M and G were secondary and tertiary contributors; except for LV in which G was a larger moderator. High input practices increased yield (4206 kg ha<sup>-1</sup>) compared to farmer practice (3347 kg ha<sup>-1</sup>) suggesting a yield gap of 859 kg ha<sup>-1</sup>. Management intensities receiving foliar fungicides improved grain properties related to milling characteristics (i.e., TKW and TWT), while management intensities receiving more nitrogen improved baking characteristics (e.g., WA and DS). Across sources of variation, yield response to improved management associated positively with the responses of TKW, TWT, and in some

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cases, GP, and WA. Our results showed the possibility of simultaneously improving grain yield and selected milling and baking attributes of bread wheat genotypes through intensive management.

### 3.1 Introduction

Wheat (*Triticum aestivum* L.) is one of the oldest cultivated grains (Uthayakumaran & Wrigley, 2017), and it is grown in environments ranging from the equator to temperate lands (Peña-Bautista et al., 2017). Globally about 760 million metric tons of wheat are harvested annually (FAOSTAT, 2021). Nearly 20% of the calories and protein demands of the world's population are supported by diverse products made from wheat (Hernández-Espinosa et al., 2018). There is large genetic diversity in wheat with more than 25,000 cultivars worldwide varying in yield potential (Lollato et al., 2020) and physical and compositional grain characteristics (Peña-Bautista et al., 2017).

On an annual basis, the United States (US) accounts for approximately 7-9% of the global wheat production and around 11% of global exports (FAOSTAT, 2021). Kansas is the largest wheat producing state in the US, producing 7-13 MMt from an area of 3.0–4.3 Mha (2006 - 2022) and exporting roughly half of its production (USDA-NASS, 2021). Despite its importance within the US and the global scenarios, Kansas still has wheat yields ( $\sim 3 \text{ Mg ha}^{-1}$ ) that are well below their potential i.e. 5.0-5.5  $\text{Mg ha}^{-1}$  (Lollato et al., 2017), resulting in a large yield gap (i.e., the difference between actual and potential yields). These large yield gaps were confirmed at the experimental (de Oliveira Silva et al., 2020; Jaenisch et al., 2019, 2022; Lollato & Edwards, 2015) and field levels (Jaenisch et al., 2021; Lollato et al., 2019a), and can be narrowed by management (Munaro et al., 2020). However, there have been no attempts to

understand whether narrowing yield gaps through improved management impact the end use quality of the wheat grain.

Increases in grain yield often decrease grain protein concentration (GP; Simmonds, 1995) owing to a dilution in GP at greater yields – if not accompanied by equivalent increases in grain N (Barneix, 2007). Recent evidence, however, suggested that it is possible to increase yield and GP simultaneously through N management (Lollato et al., 2021). Still, the end use quality of wheat is determined by many parameters beyond GP, such as flour yield and quality, as well as dough rheological properties (Corassa et al., 2018). The majority of the preliminary work on wheat yield and milling and baking quality evaluated the effects of genotype (G), environment (E), and the  $G \times E$  interaction (Souza et al., 2004; Vazquez et al., 2019; Vázquez et al., 2012; Yong et al., 2004). With rare exceptions (e.g., Rozbicki et al., 2015; Tian et al., 2022), however, the effect of crop management has been overlooked. Thus, at question here is whether improving yield through management intensification can also improve wheat milling and baking quality parameters.

Even though the relative influence of  $G \times E$  on various quality traits have been studied, there is no general agreement on which are major drivers. G has been reported to affect kernel hardness, flour yield, Zeleny sedimentation value, and arabinoxylans - non-starch polysaccharides (Finnie et al., 2006; Yong et al., 2004), but the relative importance of G, E, and  $G \times E$  varied with respect to the tested genotype and environment (Li et al., 2013). Other parameters were more dependent on E, including grain yield, thousand kernel weight (TKW), test weight (TWT), falling number (FNV), GP, flour ash (FA), total phenolic content and phytochemicals of wheat grain (Caffe-Treml et al., 2011; Hernández-Espinosa et al., 2018; Rozbicki et al., 2015; Tian et al., 2021; Yong et al., 2004). The effect of M seems to be greater

on sedimentation value, but its interaction with G can impact flour ash content substantially (Rozbicki et al., 2015).

Breadmaking quality of wheat is attributed to gluten protein (Park et al., 2006). Protein concentration of wheat is dependent on the E (Rozbicki et al., 2015; Yong et al., 2004), whereas the quality of protein i.e., protein composition, the glutenin - gliadin ratio, SDS value etc. are more dependent on G (Caffe-Treml et al., 2011; Finney, 1985; Hernández-Espinosa et al., 2018). When hydrated, these proteins form gluten which determines the rheological properties of the dough. While rheological properties are predominantly affected by G; the E and their interactions also play a major role in their determination (Williams, O'Brien, et al., 2008; Yong et al., 2004). Some preliminary evidence also suggested the role of M on maintaining or improving wheat grain quality (Torrion & Stougaard, 2017; Zecevic et al., 2010). For instance, GP is directly influenced by N management (Daaloul Bouacha et al., 2014; Lollato et al., 2019b, 2021; Vazquez et al., 2019) and increased levels of N available usually increases wheat GP (Mohammed et al., 2013) and wet gluten content (Zecevic et al., 2010). The increase in GP increases gliadin-glutenin ratio (Triboi et al., 2000) and thereby, the wheat baking quality. Nitrogen application timing also has the potential to improve GP (Corassa et al., 2018; Lollato et al., 2021), with late season N applications (i.e., around anthesis) being a fine-tuning mechanism for modest gains in GP (Cruppe et al., 2017; Giordano et al., 2022). Nitrogen also interacts with S fertilization and can impact grain asparagine concentration (Wilson et al., 2020). Another important management impacting wheat yield is the use of foliar fungicides (Cruppe et al., 2021). The combination of increased N rates and foliar fungicide can maintain GP despite improvements in yield (de Oliveira Silva et al., 2020; Fleitas et al., 2018) due to an increased leaf

area duration and prolonged N uptake and translocation (Schierenbeck et al., 2019; de Oliveira Silva et al., 2021).

While there is some general consensus that E factors such as moderate temperature during the grain filling period, relative humidity, and soil moisture availability, can improve grain yield and quality (Graybosch et al., 1995; Peña-Bautista et al., 2017; Torrion & Stougaard, 2017), a detailed analysis of the weather experienced during different developmental windows of the wheat crop on grain quality attributes is lacking. This is important because different developmental windows determine wheat yield components. For example, the time surrounding anthesis determine wheat kernel number (Fischer, 1985), while the time from booting to anthesis (Calderini et al., 2001) and from anthesis to maturity (Bergkamp et al., 2018) determine wheat kernel weight. The importance of E conditions during these periods on yield determination is well established (e.g., Cossani and Sadras, 2021; Sadras et al., 2022); however, their effects on wheat milling and baking quality attributes are not, which is partially the focus of this manuscript.

Exploiting the synergism between G, E, and M can contribute to improvements in the quality of wheat (Rozbicki et al., 2015), which is not only relevant to breeding programs, but to all wheat stakeholders (Hernández-Espinosa et al., 2018) including: farmers (grain yield), millers (test weight and flour yield), bakers (grain protein content and protein quality), and finally consumers (bread loaf and nutritional quality). Thus, this research was designed to test whether improvements in M and G that potentially narrow yield gaps would also benefit wheat milling and baking parameters. Our specific objectives were to: (i) quantify the modulation of wheat milling and baking characteristics as affected by the weather experienced during different developmental windows of the wheat crop; (ii) determine the contribution of G, E, M, and their

interactions on wheat yield, milling, and baking quality, (iii) explore associations among yield, milling, and baking quality attributes, and (iv) determine if managing for reduced yield gaps improved quality.

## **3.2 Materials and Methods**

### **3.2.1 Field experiment**

Field experiments were conducted in six environments resulting from the combination of four Kansas locations and three growing seasons (i.e., the harvest years of 2017, 2018, and 2019). Experimental locations were Ashland Bottoms (ASB, 37°11'N, 99°46'W) on a Wymore silty clay loam (fine, smectitic, mesic Aquertic Argiudol), Belleville (BEL, 39°48'N, 97°48'W) on a Crete silt loam (fine, smectitic, mesic Pachic Udertic Argiustol), Hutchinson (HUT, 37°55'N, 98°1'W) on a Ost loam (fine-loamy, mixed, superactive, mesic Udic Argiustol), and Manhattan (MAN, 39°12'N, 96°35'W) on a Kaloha silt loam (fine-silty, mixed, superactive, mesic Cimilic Hapludol).

Field experiments were a factorial combination of five genotypes (main plot) by four crop management levels (subplots) in a split-plot design with four replicates. Five hard red winter wheat genotypes including WB4269, WB4303, WB4458, WB4515, and WB-Grainfield were selected to represent: (i) different stabilities in response to management and different yield potentials (greater expected response to fungicide by the genotypes WB4303, WB4458, and WB-Grainfield due to greater susceptibility to a range of diseases; and greater tolerance to high N rates by the genotypes WB4303 and WB4269 due to better standability) (de Oliveira Silva et al., 2020); (ii) slightly different maturities for anthesis (2-8 days difference) allowing us to explore environmental interactions; and (iii) a range in protein content and quality profiles (WB4303, poor milling but good baking quality; WB4515, good milling and baking qualities; WB4269,

poor baking quality; WB4458 and WB-Grainfield, good milling and average baking qualities). Although all genotypes derived from the same breeding program, we note that they did not share direct parentage (Supplemental Table S1) thus contributing to the genetic diversity of the study which was naturally constricted by the market class and adaptation area. These genotypes occupied from 0.3 to 6.4% of the winter wheat area in the state in any given year during 2016-2022 (Supplemental Table S1).

Management levels evaluated were designed based on a previous experiment where N and fungicide were the leading causes of yield gaps in Kansas (Jaenisch et al., 2019). Management levels included: (i) farmer practice, where N rate was applied as urea (460 g N kg<sup>-1</sup>) at Feekes 4 to match a yield goal of ~4,000 kg ha<sup>-1</sup>; (ii) high-input, where the total N supplied was enough for a yield goal of 7,700 kg ha<sup>-1</sup>, in addition to 22 kg S ha<sup>-1</sup> (applied as gypsum), 45 kg Cl ha<sup>-1</sup> and 50 kg K ha<sup>-1</sup> (applied as KCl), two fungicide applications (63 g ha<sup>-1</sup> Picoxystrobin-Class 11 when the earliest maturing variety achieved jointing, and 85 g ha<sup>-1</sup> Picoxystrobin-Class 11 plus 34 g ha<sup>-1</sup> Cyproconazole-Class 3 when the earliest maturing variety achieved anthesis), and plant growth regulator (250 g ha<sup>-1</sup> as trinexapac-ethyl) applied at jointing; (iii) the high-input management however using the same N regime as the farmer practice; and (iv) the high-input management however without foliar fungicide. The latter two intensities allowed for the direct quantification of the impacts of N and fungicides, while the comparison between the current- and high-input systems allowed to quantify the current yield gap. All experimental units were sown at 84 kg of seed ha<sup>-1</sup>, received 56 kg ha<sup>-1</sup> diammonium phosphate in-furrow at sowing, and weeds and insects were controlled as needed using commercially available products. Nitrogen rates were calculated for each environment using a 30 kg N per 1000 kg ha<sup>-1</sup> yield goal, subtracting from the total N needs the (i) nitrate-N available in

the soil profile at sowing at the 0-60 cm depth, and (ii) 11 kg N ha<sup>-1</sup> for each percent organic matter in the 0-15 cm depth (Leikam et al., 2003). While actual N rates varied among environments (Supplemental Table S2 and S3), the total N available for the plots with 4,000 kg ha<sup>-1</sup> yield goal was about 130 kg N ha<sup>-1</sup>, and another 107 kg N ha<sup>-1</sup> was applied to the plots with 7,700 kg ha<sup>-1</sup> yield goal. Soil available NO<sub>3</sub>-N is provided in Supplementary Table S2 and dates for relevant field operations are provided in Supplementary Table S3.

### **3.2.2 Measurements**

The environmental characterization consisted of soil and weather variables. Fifteen individual soil cores were collected at sowing from the 0-15 and 15-60 cm depths in each environment. Samples were mixed into a composite sample, which was submitted for soil fertility and textural analyses at Kansas State University's soil fertility laboratory (Supplemental Table S2). Weather data for maximum (T<sub>max</sub>), mean (T<sub>mean</sub>), and minimum (T<sub>min</sub>) air temperature, precipitation, grass-based Penman-Monteith reference evapotranspiration (E<sub>To</sub>), and solar radiation were collected from nearby weather monitoring stations pertaining to the Kansas Mesonet (Patrignani et al., 2020), which were located no more than 500 m from the field experiments. Weather variables were then averaged (T<sub>max</sub>, T<sub>min</sub>, T<sub>mean</sub>, and solar radiation) or accumulated (precipitation and E<sub>To</sub>) for relevant portions of the crop cycle, including: (i) the full growing season from sowing to harvest, (ii) the critical period for yield determination from 300 °C prior to Feekes 10.5 to 100 °Cd afterwards using a base temperature of 4.5°C (Fischer, 1985), and (iii) the grain filling period from 100 °C until 600 °Cd after Feekes 10.5 using a base temperature of 0 °C (Dupont et al., 2006). The duration of each period was calculated in number of days. We also calculated the ratio of accumulated precipitation over E<sub>To</sub>, as an indicative of

seasonal water supply to water demand ratio (WS: WD); and the photothermal quotient (PTQ, the ratio of solar radiation and temperature).

Grain yield was measured at harvest maturity using a Massey Ferguson 8XP auto-propelled small plot combine by harvesting the entire experimental unit, with a harvested area of approximately 16 m<sup>2</sup> (experimental units were seven 19 cm spaced rows and 10 m long). Grain samples from wheat harvest were maintained separate by experimental unit for analyses of grain quality traits, totaling 480 samples. Grain test weight (TWT) was determined by standard procedure (AACC 55 – 10.01) with test weight scale (Seedburo Equipment Company, Des Plaines, IL, USA), and a thousand kernel weight (TKW) was measured with an electronic seed counter.

Wheat grains were tempered to 15-16% moisture content, wet basis (AACC Method 26 – 10.02) and milled with a Brabender Quadrumat Senior mill (AACC 26 – 21A). The percentage of flour obtained from a given amount of wheat on milling was expressed as flour yield (FY) (Schuler et al., 1995). Protein content (GP) was determined by Kjeldhal method following standard AACC procedure (12% moisture wet basis, AACC 46-30.01). Hagberg falling number (FNV) was measured following the method AACC 56-81.04 using Falling Number System (Model: Alphatec FNo, Make: Foss, Denmark) with the amount of flour as specified on standard protocol [based on moisture content (wet basis, %)] used for analysis. Uniform suspension of flour was formed by adding 25 ml of water to the sample in the viscometer tube and shaking it vigorously for 20-30 times. The viscometer tube with an inserted stirrer was placed in the boiling water bath of the falling number system. Time taken by the stirrer to reach the bottom of the gelatinized suspension was the falling number. Flour ash was analyzed by AACC 08 – 01.01 (AACC Methods, 2011).

Dough characteristics were measured with the Farinograph (AACC 54 – 21.02) for evaluating water absorption, mixing tolerance index, and stability. Water absorption or hydration capacity was defined as the quantity of water absorbed by 300g of flour to obtain dough of standard consistency (500 BU). Dough development time (DDT) is the time between first addition of water to development of dough maximum consistency. Mixing tolerance index (MTI) represents the tolerance of the dough to mixing. Hard wheat flour with  $MTI \leq 30$  BU is considered good whereas, those above 50 BU are weak flour. Dough stability (DS) measured in minutes is the difference between arrival time (time at which top of the curve first intercepts the 500 BU line) and departure time (time at which top of curve leaves the 500 BU line). Baking quality evaluations involved standard pound loaf test (AACC 10 – 11.01). The bread formula for the analysis consisted of 700 g flour, 17.5 g yeast, 35 g sugar, 14 g salt and 21 g shortening. The baked loaves were analyzed for loaf volume following the rapeseed displacement method (AACC 10 – 05.01).

### **3.2.3 Statistical analysis**

The impact of weather variables during the three phases described above on crop yield and milling and baking characteristics were evaluated using Pearson's correlation analysis. Variability in the measured traits was examined using descriptive statistics such as mean, minimum, maximum, standard deviation (SD), and coefficient of variability (CV) (Table 2). Variance component analysis estimated the share of factors and their interaction on total variability by residual maximum likelihood (Williams, Brien, et al., 2008) using the PROC VARCOMP in SAS 9.4 (SAS Institute Inc., 2021) with G, E, M and their interactions as

random factors. The variance components were presented as percentage of total variance (e.g., Rozbicki et al. 2015).

Three-way analysis of variance (ANOVA) considering G, E, M, and their interactions as fixed effects, and replication nested within E as well as G nested within replication and E as random effects, determined the significance of the evaluated factors on yield and quality traits. The ANOVA was performed through PROC GLIMMIX procedure in SAS 9.4. For traits exhibiting significant two- or three-way interactions, responses were explored through adaptability and stability analysis following the method proposed by Eberhart & Russell (1966). Here, a linear regression analysis (Eq. 3.1) was performed on the individual treatment response as function of an environmental index for that respective response (I, Eq.3. 2), which was calculated as the difference between the measured traits for that particular G-E-M combination and the overall grand mean for that trait. The output of this analysis includes an adaptability index (i.e., the slope of the relationship), a stability index (i.e., the model fit statistics), and the mean trait value:

$$Y_{ij} = \beta + \alpha I_j + \delta_{ij}$$

where  $Y_{ij}$  is the observation of the  $i$ th genotype in the  $j$ th environment;  $\beta$  is the general mean of the  $i$ th genotype over all environments,  $\alpha$  is the regression coefficient that measures the response of  $i$ th genotype to different environments and  $\delta_{ij}$  is the deviation from regression of the  $i$ th genotype in the  $j$ th environment,  $I_j$  is the environmental index (Nascimento et al., 2021)

$$I_j = \frac{\sum_i Y_{ij}}{g} - \frac{\sum_i \sum_j Y_{ij}}{ga}$$

The relationships among the analyzed traits were evaluated through principal component analysis.

Genotype-specific trait response to M was calculated by subtracting the mean in the standard management control from the mean of each of the management intensification regimes within environment. We then evaluated the relationships among quality trait difference and yield difference at each step in management intensification using regression analysis to understand whether modulation in yield related to modulation of quality traits (e.g., Slafer et al., 2014, 2022)

### **3.3 Results**

#### **3.3.1 Weather conditions and their impact on measured variables**

Growing season thermal time accumulation ranged from 2094 °C in ASB19 and BEL18, to 2702 °C in HUT17, and growing season length ranged from 244 to 252 days (Fig. 3.1). Growing season precipitation ranged from 273 mm in BEL18 to 723 mm in MAN19 and growing season ETo ranged from 622 mm in MAN19 to 790 mm in HUT17 (Fig. 3.1), with WS:WD ratio ranging from 0.38 to 1.16. Duration of the critical period ranged from 24 to 48 days, with associated Tmean ranging from 12.9 to 21.1 °C and WS: WD from 0.12 to 2.83. Grain filling duration ranged from 18 to 26 days with associated Tmean ranging from 19.1 to 25.2 °C and WS: WD from 0.31 to 1.38.

Weather variables experienced in the critical period modulated grain yield and most quality parameters more strongly than those experienced in grain filling or during the entire season, although Tmean and solar radiation in the grain filling period related positively with a number of flour quality parameters (Table 3.1). Precipitation, the ratio of water supply-to-water demand, and the duration of the critical period related positively to grain yield while Tmean and solar radiation related negatively. Test weight was strongly and positively related to PTQ and ETo during the critical period. Grain protein, FP, FNV, and farinograph peak related positively to Tmean and solar radiation in the critical period and in the grain filling period, and negatively

with duration of both periods, PTQ and ETo in the critical period. The duration of the critical period and of the grain filling period (in number of days) impacted MTI positively, while Tmean and solar radiation impacted MTI negatively. These correlations were opposite for DS.

### **3.3.2 Grain yield, yield gaps, and yield stability**

Grain yield varied mostly with respect to E (2703 – 5117 kg ha<sup>-1</sup>) followed by M (3345 – 4206 kg ha<sup>-1</sup>) and lastly by G (3341 – 3983 kg ha<sup>-1</sup>) (Table 3.2), also supported by the variance component analysis that suggested that E explained 51% of yield variability, M and its interaction with E 22%, and lastly G and its interaction with E 10% (Table 3.3). Grain yield was highest in HUT19 (5097 kg ha<sup>-1</sup>) and lowest in ASB19 (2703 kg ha<sup>-1</sup>), with other locations showing intermediate yields owing to location-specific characteristics such as soil, sowing dates, and weather conditions.

The E × M and the E × G interactions for yield are depicted in Fig. 3.2A and 3.2B, with associate regression coefficients in Tables 3.4 and 3.5. Grain yield differences among M intensities were most apparent in high yielding E (Fig. 3.2A). The farmer practice had a broad adaptability ( $\alpha = 1$ ) with mean grain yield of 3347 kg ha<sup>-1</sup>. Meanwhile, the high input system had adaptability specific to high-yielding E ( $\alpha > 1$ ) and a mean grain yield of 4206 kg ha<sup>-1</sup>, suggesting an overall yield gap of 859 kg ha<sup>-1</sup> and larger gaps in higher yielding E. The high-input minus N had a similar adaptability to that of the standard control but at a greater mean yield level (4006 kg ha<sup>-1</sup>), while the high-input minus fungicide showed adaptability specific to low yielding E ( $\alpha < 1$ ) and mean yield similar to the control (3385 kg ha<sup>-1</sup>). Grain yield differences among genotypes was more apparent in low-yielding E (Fig. 3.2B). While the genotype WB4269 had the highest mean yield (3983 kg ha<sup>-1</sup>), it also had adaptability specific to low-yielding E ( $\alpha < 1$ ) and relatively low stability ( $r^2 = 0.82$ ). The other genotypes had broad

adaptability ( $\alpha = 1$ ) with mean grain yield ranging from 3328 (WB4458) to 3972 (WB-Grainfield) and stability coefficients ( $r^2$ ) from 0.84 and 0.93.

### 3.3.3 Grain quality

There was a wider variability for TWT among E (71.7 – 78.2 kg hl<sup>-1</sup>, 37% variability) as compared to G (74.0 – 78.1 kg hl<sup>-1</sup>, 28%) or M (74.6 – 77.4 kg hl<sup>-1</sup>, 17%) (Tables 3.2 and 3.3). Foliar fungicides were largest determinants of TWT as the lowest means occurred in the farmer practice and high minus fungicide treatments (72.9 and 72.7 kg hl<sup>-1</sup>) (Table 3.4). The genotype WB4515 had the highest mean TWT (76.1 kg hl<sup>-1</sup>) with broad adaptability ( $\alpha = 1$ ) with relatively high stability ( $r^2 = 0.95$ ), while WB4303 was the opposite (mean: 72 kg hl<sup>-1</sup>,  $\alpha = 0.72$ ,  $r^2 = 0.84$ ) (Table 5). The range of TKW was broader for E (21.7 to 30.3 g, 55%) than for G (25.4 to 28.8 g, 18%) or M (25.4 to 28.4 g, 15%) (Tables 3.2 and 3.3). Similarly, to grain TWT, TKW was highest in treatment receiving foliar fungicides (27.7-28.4 g *versus* 25.4-26.4 g) which also resulted in broad adaptability ( $\alpha = 1$ ) (Table 3.4). The genotypes WB4458 and WB4303 had the highest TKW though with contrasting adaptabilities ( $\alpha = 1.34$  *versus* 0.77, respectively) and stabilities ( $r^2 = 0.94$  *versus* 0.85).

### 3.3.4 Milling and flour quality

GP associated more with E (65% of GP variability; range: 10.3 – 16.6%) than with M and M  $\times$  E (20% of GP variability, range: 12.2 – 14.2%) or G and G  $\times$  E (9% of GP variability; range: 12.5 – 13.7%) (Tables 3.2 and 3.3). GP as high as 16% occurred in BEL18. The high-input and the high-input minus fungicide treatments had greater GP as compared to farmer practice or to the high input minus N treatment (Table 3.4). However, the GP in these treatments with high mean GP were adaptable to low GP environments ( $\alpha < 1$ ) suggesting that their benefit decreased as

mean GP increased (Table 3.4). Also, the studied genotypes had stable GP content ( $r^2 \geq 0.97$ ) in all environments though mean GP was lower in WB4269 and WB-Grainfield (Table 3.5).

E contributed significantly to the variation in wheat FNV (25%), which ranged from 309 to 688 s. While M and M  $\times$  E only accounted for 5% of the variability in FNV, the average FNV was highest (483 s) for the high input and the high input minus fungicide treatments, and lowest for the farmer practice (474 s) and high minus N treatments (466 s) (Table 4). The lowest FNV treatments also had adaptability specific to high FNV environments ( $\alpha > 1$ ) and high stability ( $r^2 = 0.98$ ) (Table 3.4). G and G  $\times$  E interaction also had minimal contribution to FNV (4%) (Table 3.3). WB-Grainfield and WB4269 had the highest FNV (483-486 s) and broad adaptability ( $\alpha = 1$ ), although WB4269 had lower stability ( $r^2 = 0.85$  versus 0.64). The mean FNV (464 s) was the lowest for WB4515, although it had adaptability specific to high FNV environments (Table 3.5).

Flour yield varied between 68 and 72%, with E accounting for a significant proportion of its variability (35%) and very low variability attributed to M (Table 3.3), with all M practices resulting in broad adaptability (Table 3.4). About 13% of FY variability was attributed to G and G  $\times$  E (Table 3.3). WB-Grainfield and WB4515 had high mean FY (71%) but differed in adaptability, as the former had broad adaptability ( $\alpha = 1$ ) and the latter had adaptability specific to high FY environments (Table 3.5). Flour ash content varied greatly with E (45%). G and G  $\times$  E accounted for 10% of the variation in FA; M and M  $\times$  E had a share of 7% in the variation (Table 3.3). The range in FA was narrow and only went from 0.51-0.54 (Tables 3.4, 3.5).

### **3.3.5 Dough rheology and baking**

E was a major contributor to WA (66%), while G and G  $\times$  E (9%), and M and M  $\times$  E (8%) were minor contributors. While the influence of E was smaller for other rheological properties of the flour, such as farinograph peak (43%), MTI (28%), and farinograph stability (36%), it was still

the largest contributor their variability. G and G  $\times$  E accounted for 9, 21, and 22% and M and M  $\times$  E accounted for 16, 8, and 13% of the variability in farinograph peak, MTI, and stability (Table 3.3). Other dough characteristics like DDT and DS were also influenced by the E (49-61%), and G and G  $\times$  E (17 – 30%); meanwhile M and M  $\times$  E had greater influence on DDT (32%) as compared to LV (6%). Bread LV from BEL18 was the lowest, which can be related to the higher water absorption of these samples. The variation among the LV was greatest for bread from HUT17.

The high minus N management and farmer practice resulted in WA adaptability specific to high WA environments ( $\alpha > 1$ ). The highest mean WA resulted from the High input treatment (59.6%) though the adaptability was specific to low WA environments ( $\alpha < 1$ ). The genotype WB-Grainfield had WA adaptability specific to high WA environments ( $\alpha > 1$ ). DDT varied between 5-7 min for the genotypes grown in different environments, and high minus N treatment improved the adaptability of the genotypes to high DDT environments. WB-Grainfield and WB4303 represented greater mean values in terms of rheological properties like WA (58.2 and 59.6%, respectively), DDT (5.3 and 6.2 min, respectively), MTI (30.7 and 28.54 BU, respectively) and DS (10.5 and 12.6 min, respectively). The high bread loaf volume environments ( $\alpha > 1$ ) favored genotypes WB 4269 and WB 4458 though it was not favorable for other rheological parameters.

The PCA suggested that the percentage of total variation of the dataset among the combinations explained by PC1 and PC2 was 33.5 and 18.6% (Fig. 3.3A), with the first four components explaining nearly 72.6% variation in the data. PC1 was positively correlated with GP, FNV, WA, and DS, and negatively correlated with MT, while PC2 was positively correlated with TWT, FY and TKW. GY had a strong positive correlation with PC4. The effect of different

E on the bread making quality of the winter wheat are presented in Fig. 3.3B. The traits that were strongly correlated with E (i.e., GP, FNV, and DS) had the highest correlation with PC1. For samples from BEL18, the mean values for GP, FNV, WA, DS and LV were highest for the flour whereas lowest for MTI which implies that the flour and baking quality were better.

### **3.3.6 Improving yield and functionality simultaneously**

Across all sources of variation and within G and E, the response of GY from the farmer practice to high input ranged from -172 to 2589 kg ha<sup>-1</sup> and was positively associated the responses of TKW (range: -2 to 6.3 kg hl<sup>-1</sup>), GP (range: 0.4 to 3.2%), and WA (range: 0 to 4.8%) (Fig. 3.4a-c). There were no other associations between GY response and the response of other quality traits. A similar analysis but constrained to the high input minus nitrogen treatment suggested that increases in GY (range: -95 to 1997 kg ha<sup>-1</sup>) associated positively with increases in TWT (range: 0.4 to 6.4 kg hl<sup>-1</sup>) and TKW (range: -2.2 to 5.7 g) (Fig. 3.4 d, e), and negatively with FA (range: 0.03 to -0.1%) (Fig. 4f). When all inputs were provided except for fungicides, increases in GY (range: -1145 to 1182 kg ha<sup>-1</sup>) associated positively with increases in TWT (range: -1.4 to 2.6 kg hl<sup>-1</sup>) and TKW (range: -2.9 to 1.4 g) (Fig 3.4g, h), and negatively with FA (range: -0.04 to 0.04%), FNT (-49 to 65 s), MTI (range: -27 to 10 BU), and DD (range: -2.5 to 8.8 min) (Fig. 3.4i-l).

## **3.4 Discussion**

Data from 480 wheat grain samples revealed G, E, and M factors modulating grain yield and milling and baking quality. We ensured that the levels of E, G, and M conditions evaluated were within the typical conditions experienced by Kansas wheat growers: Three contrasting growing seasons provided environmental variability to represent long-term weather variability (Lollato et

al., 2017; 2020); management practices represented different levels of management intensification within the range of currently adopted practices in commercial wheat fields in the region (Jaenisch et al., 2021; Lollato et al., 2019a); and the genotypes evaluated are commercially available and have occupied substantial proportion of the wheat area within Kansas (Supplemental Table S1). The results from this research suggested that most variables were highly dependent on the main effects of E, M, and G, and to a lesser extent on their interactions. Among the interactions,  $E \times M$  and  $E \times G$  explained greater proportion of the variability of most traits as compared to  $G \times M$  or the three-way interaction. We showed that a significant yield gap of winter wheat exists, and that improved agronomic management can narrow these gaps. An original contribution of this research is the opportunity to improve both yield and quality traits simultaneously, which to some extent challenges the status quo that wheat yield and quality are necessarily negatively related.

### **3.4.1 Environment**

Some authors consider the perception of environment as “ambiguous” (Vázquez et al., 2012) owing to its different interpretation. For example, agro-ecological zones considering similarities in soil and weather have been considered environment (e.g., Rattalino Edreira et al., 2017); for others, the term encompasses not only soil characteristics and climatic conditions but also technical interventions here referred to as ‘management’ (Hernández-Espinosa et al., 2018), and finally certain authors consider location and year effects independently (Rozbicki et al., 2015) without consensus on how to treat them statistically (e.g., fixed or random effects; Moore & Dixon, 2015). We were not able to differentiate the effects of year and location due to the unstructured nature of the environments evaluated (i.e., different locations studied different years), thus using a single variable “environment”. The benefit of this approach is that it

considers the weather conditions experienced in each combination of location and year as an environment because the quantitative soil and weather conditions during the crop season regulate crop growth and yield, while the nominal variables ‘location’ and ‘year’ are biologically uninformative (Sadras et al., 2017).

Recent efforts evaluated probabilistic patterns of drought (Sciarresi et al., 2019) and of the combination of drought and thermal regime stresses (Couëdel et al., 2021; Lollato et al., 2017, 2020) for winter wheat in the U.S. Great Plains, overwhelmingly concluding that grain yield of winter wheat in this region is often impacted by heat and drought stresses. The current research expands on these previous environmental characterizations to explore functional relationships between weather experienced in the growing season and grain yield and quality traits. While these relationships are statistically sound and biologically meaningful, they imply correlation and not necessarily causation as they include underlying confounding effects (Bonada & Sadras, 2015), as suggested by Sadras et al. (2019). The significant associations between grain yield and weather variables during the critical period are supported by existing literature, such as the positive associations of yield with precipitation (Lollato et al., 2017) and duration (Cossani & Sadras, 2021), and the negative associations with Tmean (Cossani & Sadras, 2021). We note in passing that recent evidence suggests that wheat is less responsive to N applications under warmer conditions during the critical period (Sadras et al., 2022). This association between mean temperatures during the critical period and yield response to an overall intensified management, such as the one explored in the current work, is yet to be studied. The negative association of grain yield and solar radiation, while unexpected, can likely be attributed simply to lower precipitation in seasons with greater solar radiation (slope:  $-31 \text{ mm MJ}^{-1} \text{ d}^{-1}$ ,  $R^2 = 0.52$ ,  $p < 0.001$ ).

The associations of weather variables in the critical period, which occurs prior to the period of grain weight increase, with quality traits can potentially be explained due to the development of the kernel carpel (Calderini et al., 2001) and kernel number (Fischer et al., 1985) during this period, and the often-reported negative association between kernel number with kernel weight (Slafer et al., 2014). The most pronounced effect of weather variables on yield is mediated by its effect on kernel number (McCaig, 1997). Precipitation around anthesis (McCaig, 1997) and under irrigated conditions, the ratio of incoming solar radiation to temperature (Fischer, 1985), increases the number of kernels per area and positively affects yield. However, this increase in kernel number naturally originates smaller kernels as more kernels are developed in distal spikelets within the spike, and in distal florets within the spikelet – which are naturally smaller (Slafer et al., 2014; 2022). Thus, yield not always associates with kernel weight either at the regional level (de Oliveira Silva et al., 2020; Jaenisch et al., 2022) or across large global datasets (Slafer et al., 2014, 2022). The weather during the critical period seems to also determine grain quality traits in oats (*Avena sativa* L.) (Sadras et al., 2019) and grain protein response to late-season N (Giordano et al., 2022). Across all sources of variation, weather relations with GP and its associated variables (FP, FNV, and DDT, Fig. 3.2) mirrored those of grain yield and thus were favored by conditions that reduced yield, which is likely due to dilution effect (Barneix, 2007).

### **3.4.2 Grain yield and yield gaps**

Grain yield was mostly driven by E, M, and their interaction, with a smaller proportion of yield modulated by G (Table 2). These findings are similar to a previous report from a broader geography where E accounted for ~46% and M for ~32% of yield variability, with only ~2-8% accounted for by G (Munaro et al., 2020). These results highlight the importance of agronomic

interventions to increase yield, which is especially important when grain yield in farmers' fields fail to sustain historical rates in progress in many regions of the world (Grassini et al., 2013) including the study region (Patrignani et al., 2014). Also, these results provide empirical evidence to support further research and development investments in crop management to reduce the risks of not meeting future food demand. Meanwhile, the small proportion of genotypic variability on grain yield was also reported in other regions of the world (Cullis et al., 2000; Finlay et al., 2007; Friesen et al., 2016; Mohammadi et al., 2009). Within the context of the current study, this small share of yield variability explained by G is likely due to testing only adapted genotypes that have been released for commercialization after a strict development and registration process (Friesen et al., 2016), not undermining the need to continue breeding adapted genotypes.

Grain yield gaps averaged  $859 \text{ kg ha}^{-1}$ , which is similar to previous reports for this region (de Oliveira Silva et al., 2020, 2021; Jaenisch et al., 2019, 2021, 2022). While the current study considered a general improvement in management through a high-input practice and a couple of alternative practices restricting either foliar fungicides or nitrogen rates, at the farmer level such a high input may not be justifiable due to economic constraints and therefore the refinement of the recommendations should be specific to each production system (Andrade et al., 2022; Jaenisch et al., 2021). Nonetheless, through stability analysis we showed that yield gaps were larger in higher yielding seasons, suggesting a greater opportunity-cost of the farmer practice when conditions are favorable. A greater yield potential in higher yielding seasons is usually experienced not only in replicated studies (Di Mauro et al., 2022; Jaenisch et al., 2019; 2022) but also in surveys of commercial fields of wheat and other crops (Di Mauro et al., 2018; Fink et al., 2022; Jaenisch et al., 2021; Lawes et al., 2021).

### 3.4.3 Milling and baking traits as function of G, E, and M

While the evaluated traits had values that spanned the ranges normally reported for hard winter wheat, though with slightly greater range (Rozbicki et al., 2015) (Table 3.2). The greater association of GP with E and M as compared to G is similar to results by Rozbicki et al. (2015) and Williams et al. (2008). Wheat GP was mostly influenced by the E – which was evident from the positive correlation of GP with the temperature during the critical period and grain filling (Table 5). Meanwhile, the quality of the protein is typically genotype-dependent (Murray et al., 2017) – which was also evident given that 19% of the variability in bread LV originated from G (Table 3.3). We also noted that the GP varied significantly when G were grown in different environments (Souza et al., 2004) partially due to wheat phenology and developmental time (Malik et al., 2013) and potentially different nutrient uptake dynamics (Lollato et al., 2021).

There is usually a negative correlation between the GP and grain yield (Corassa et al., 2018) due to a dilution effect resulting from an increase in the grain carbohydrate content (Torrior & Stougaard, 2017), creating challenges to the baking industry as growers aim at higher yields. This is especially true as modern genotypes do not maintain similar GP levels as historical ones owing to dilution due to higher yields (Maeoka et al., 2020). Here, the high input management increased GP simultaneously with grain yield (Fig. 3.5). Similar deviation from inverse relationship between GP and yield was reported by Torrior et al. (2019) on high N treatments ( $>100 \text{ kg ha}^{-1}$ ). Also, some evidence suggests that the application of S at jointing can improve wheat GP (Habtegebrial & Singh, 2009; Cai et al., 2022). Thus, in the high input treatment, the synergistic effect of N fertilization, S application, and foliar fungicides may have contributed to positive correlation between yield and GP, which is supported by preliminary evidence where M maintained or improving wheat grain quality (Torrior & Stougaard, 2017; Zecevic et al., 2010).

Grain protein is directly influenced by nitrogen management (Daaloul Bouacha et al., 2014; Lollato et al., 2019b, 2021; Souza et al., 2022; Vazquez et al., 2019) and increased levels of nitrogen available usually increase wheat GP (Mohammed et al., 2013) and wet gluten content (Zecevic et al., 2010). Generally, increases in GP are associated with increases in  $\omega$  gliadins and high molecular weight GS but a decrease in  $\alpha$ -,  $\gamma$ - gliadins and low molecular weight GS (Xue et al., 2019). The increase in GP increases gliadin-glutenin ratio (Triboi et al., 2000) and thereby, the wheat baking quality. The combination of increased N rates and foliar fungicide applications can maintain or improve GP concomitantly with improvements in yield (Cruppe et al., 2021; de Oliveira Silva et al., 2020, 2021; Fleitas et al., 2018) due to an increased leaf area duration and prolonged N uptake and translocation (Schierenbeck et al., 2019). Thus, M invariably interfere the baking quality as it is related with flour composition especially GP composition.

Rheological properties of dough include starch and protein, and the addition of water to the flour causes the hydration of gluten with the interaction of gliadin and glutenin. These hydrated gluten networks form the framework for embedding starch granules and help in gas retention by holding the air cells. Environment and G contributed significantly to the variation in rheological properties. GP and the farinograph indices WA ( $p < 0.05$ ,  $R^2 = 0.66$ ), DDT ( $p < 0.05$ ,  $R^2 = 0.77$ ), and DS ( $p < 0.05$ ,  $R^2 = 0.60$ ) were positively related (Wilson et al., 2020), indicating a greater dough strength with increasing GP. In general, higher WA is preferred for hard wheat flour as it is associates with increased loaf volume and loaf weight, and delayed loaf staling (Mikhaylenko et al., 2000). Management practices, especially high input with N and S fertilization, improved the DS. Application of S increases the glutenin content (both low molecular weight GS and high molecular weight GS) of protein (Cai et al., 2022). Increase in low molecular weight GS improves the rheological properties of the flour. The contribution of management practices to

MTI of the flour was lower as compared to the influence of E, G, and  $E \times G$ . In the study, N management improved the rheological characteristics of the flour and thereby the baking quality.

#### **3.4.4 Improving wheat yield and functionality traits simultaneously**

To our knowledge, this is the first report exploring the associations of yield responsiveness to management with the responsiveness to management of different quality components. This approach has been used in the literature to assess physiological drivers of wheat yield (e.g., Slafer et al., 2014, 2022; de Oliveira Silva et al., 2020; Jaenisch et al., 2022); however, this is the first time the approach is used to highlight opportunities to simultaneously increase wheat yield and milling and baking quality. Management practices that improved grain yield simultaneously increased grain TKW and TWT. These qualities are associated with morphology of the grains and contribute to FY and thereby milling quality, which is expressed through FY and FA (Li & Posner, 1989). High input minus N or minus fungicide treatments both resulted in kernels with better TKW and TWT and low FA content which are desirable for milling. The ratio of bran and endosperm change with increase in yield (Murphy et al., 2008). This tradeoff causes the negative relationship between yield and FA with improved management practices (Fig. 3.4). High input practices that improved yield had a positive association with WA whereas when fungicide was removed, a negative correlation with dough rheological parameters (MTI and DDT) (Fig. 3.4). This is attributed to the dilution in gliadin content with an increase in grain yield and TKW (Landolfi et al., 2021).

### **3.5 Conclusions**

This study revealed that the primary contributor of variance in most wheat grain, milling, and baking quality attributes was E, followed by M and lastly by G – although G was a dominant determinant of bread loaf volume. While this conclusion is limited to a small pool of locally

adapted genotypes pertaining to the same commercial class, the genotypes were contrasting in genetic background and in agronomic parameters. From an environmental perspective, a novel finding from our work was that the weather variables characterizing the critical period for yield formation controlled not only grain yield but also most quality parameters more strongly than weather variables occurring during the grain filling period or during the entire season. Another novel finding of the current work is that high input management practices increased yield (consequently narrowing the yield gap) and simultaneously improved the milling and baking quality of the harvested grain. From a management perspective, these improvements resulted from a concomitant increase in milling attributes due to foliar fungicide applications (i.e., TKW, TWT, FY and reduced FA), and in baking attributes due to fertility management (i.e., increases in GP, WA, DS and LV, and a decrease in MTI). Thus, this research shows that management practices can reduce the yield gaps and improve the rheological properties of the dough and baking quality of the studied wheat genotypes.

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## Tables

**Table 3.1. Correlations between grain, milling, and baking traits for five hard red winter wheat genotypes, averaged across four management intensities, and daily average of environmental factors during different developmental windows. The combination of five genotypes of differing phenology and six environments resulted in 30 observations to originate correlations. TWT: test weight, TKW: thousand kernel weight, GP: grain protein, FY: flour yield, FA: flour ash, FP: flour protein, FNV: falling number, WA: flour water absorption, DDT: dough development time, MTI: mixing tolerance index, DS: dough stability, DMT: dough mixing time, LF: loaf volume. Tmean: mean air temperature (°C), SRAD: solar radiation (MJ m<sup>-2</sup> d<sup>-1</sup>), PTQ: photothermal quotient (MJ m<sup>-2</sup> °Cd<sup>-1</sup>), WS:WD: water supply to water demand ratio, CTT: cumulative thermal time. Red indicates negative correlations, blue indicates positive correlations. Light colors indicates significant at  $P \leq 0.05$  and dark colors indicate significant at  $P \leq 0.01$ .**

| Environ. factor | Develop. window   | Yield<br>(kg ha <sup>-1</sup> ) | TWT<br>(kg hl <sup>-1</sup> ) | TKW<br>(g) | GP<br>(%) | FY<br>(%) | FA<br>(%) | FP<br>(%) | FNV<br>(s) | WA<br>(%) | DDT<br>(min) | MTI<br>(BU) | DS<br>(min) | DMT<br>(min) | LF<br>(cm <sup>3</sup> ) |
|-----------------|-------------------|---------------------------------|-------------------------------|------------|-----------|-----------|-----------|-----------|------------|-----------|--------------|-------------|-------------|--------------|--------------------------|
| Tmean           | Sowing to harvest | -0.07                           | 0.16                          | 0.34       | -0.71     | 0.19      | -0.68     | -0.75     | -0.74      | -0.33     | -0.71        | 0.56        | -0.58       | -0.24        | 0.21                     |
| SRAD            | Sowing to harvest | -0.37                           | 0.31                          | 0.08       | 0.35      | 0.19      | 0.18      | 0.38      | 0.63       | 0.28      | 0.44         | -0.21       | 0.29        | 0.21         | -0.30                    |
| Precip.         | Sowing to harvest | 0.18                            | -0.30                         | -0.44      | -0.34     | -0.71     | 0.62      | -0.32     | -0.24      | -0.75     | -0.32        | 0.00        | 0.08        | -0.49        | 0.44                     |
| PTQ             | Sowing to harvest | -0.10                           | 0.00                          | -0.21      | 0.71      | -0.04     | 0.56      | 0.75      | 0.83       | 0.41      | 0.74         | -0.52       | 0.56        | 0.30         | -0.29                    |
| WS:WD           | Sowing to harvest | 0.15                            | -0.35                         | -0.50      | -0.23     | -0.72     | 0.66      | -0.21     | -0.16      | -0.69     | -0.23        | -0.10       | 0.17        | -0.41        | 0.45                     |
| CTT             | Sowing to harvest | -0.08                           | 0.11                          | 0.29       | -0.69     | 0.17      | -0.64     | -0.72     | -0.72      | -0.27     | -0.69        | 0.61        | -0.65       | -0.28        | 0.11                     |
| Eto             | Sowing to harvest | 0.01                            | 0.46                          | 0.57       | -0.24     | 0.58      | -0.64     | -0.25     | -0.15      | 0.35      | -0.15        | 0.47        | -0.50       | -0.05        | -0.47                    |
| Duration        | Sowing to harvest | 0.53                            | -0.13                         | -0.01      | 0.13      | 0.02      | 0.12      | 0.17      | 0.04       | 0.44      | 0.16         | 0.19        | -0.29       | -0.21        | -0.57                    |
| Tmean           | +100 to +600 °Cd  | -0.14                           | -0.18                         | -0.40      | 0.79      | -0.02     | 0.57      | 0.82      | 0.82       | 0.47      | 0.78         | -0.51       | 0.52        | 0.30         | -0.37                    |
| SRAD            | +100 to +600 °Cd  | -0.41                           | 0.03                          | -0.18      | 0.61      | 0.04      | 0.41      | 0.63      | 0.73       | 0.30      | 0.62         | -0.45       | 0.52        | 0.35         | -0.20                    |
| Precip.         | +100 to +600 °Cd  | -0.36                           | -0.14                         | -0.39      | 0.02      | -0.40     | 0.35      | 0.01      | 0.17       | -0.43     | -0.01        | -0.23       | 0.31        | -0.04        | 0.39                     |
| PTQ             | +100 to +600 °Cd  | -0.42                           | 0.33                          | 0.34       | -0.24     | 0.13      | -0.26     | -0.26     | -0.12      | -0.23     | -0.22        | 0.09        | 0.01        | 0.11         | 0.24                     |
| WS:WD           | +100 to +600 °Cd  | -0.28                           | -0.17                         | -0.43      | -0.01     | -0.40     | 0.35      | -0.02     | 0.13       | -0.46     | -0.03        | -0.24       | 0.30        | -0.08        | 0.40                     |
| ETo             | +100 to +600 °Cd  | -0.35                           | 0.27                          | 0.34       | 0.09      | 0.26      | -0.22     | 0.09      | 0.21       | 0.37      | 0.11         | 0.21        | -0.17       | 0.16         | -0.34                    |
| Duration        | +100 to +600 °Cd  | 0.14                            | 0.20                          | 0.47       | -0.69     | 0.04      | -0.59     | -0.72     | -0.74      | -0.34     | -0.69        | 0.49        | -0.50       | -0.21        | 0.32                     |
| Tmean           | -300 to +100 °C   | -0.41                           | -0.21                         | -0.44      | 0.75      | -0.02     | 0.51      | 0.77      | 0.77       | 0.36      | 0.71         | -0.53       | 0.56        | 0.35         | -0.23                    |
| SRAD            | -300 to +100 °C   | -0.46                           | 0.08                          | -0.21      | 0.66      | 0.21      | 0.29      | 0.67      | 0.80       | 0.41      | 0.69         | -0.45       | 0.50        | 0.38         | -0.27                    |
| Precip.         | -300 to +100 °C   | 0.68                            | -0.04                         | 0.05       | -0.55     | -0.40     | 0.18      | -0.52     | -0.53      | -0.54     | -0.47        | 0.26        | -0.25       | -0.56        | 0.20                     |
| PTQ             | -300 to +100 °C   | -0.04                           | 0.68                          | 0.63       | -0.37     | 0.51      | -0.60     | -0.37     | -0.09      | 0.06      | -0.20        | 0.32        | -0.28       | -0.02        | -0.09                    |
| WS:WD           | -300 to +100 °C   | 0.64                            | -0.17                         | -0.09      | -0.43     | -0.48     | 0.32      | -0.41     | -0.46      | -0.55     | -0.39        | 0.16        | -0.14       | -0.52        | 0.23                     |
| ETo             | -300 to +100 °C   | 0.05                            | 0.53                          | 0.62       | -0.41     | 0.52      | -0.77     | -0.43     | -0.28      | 0.18      | -0.30        | 0.42        | -0.46       | 0.02         | -0.15                    |
| Duration        | -300 to +100 °C   | 0.38                            | 0.28                          | 0.49       | -0.77     | 0.10      | -0.56     | -0.78     | -0.73      | -0.31     | -0.70        | 0.58        | -0.61       | -0.36        | 0.13                     |

**Table 3.2. Descriptive statistics of yield, milling, and baking quality traits of five hard red winter wheat genotypes grown in six Kansas environments and exposed to four levels of management intensities. Data presented for one source of variation (e.g., environment) was calculated across the other sources of variation (e.g., management and genotype). Min.: minimum, Max.: maximum, SD: standard deviation, CV: coefficient of variation**

| Trait                        | Environment |        |        |       |      | Management |        |       |      | Genotype |        |       |      |
|------------------------------|-------------|--------|--------|-------|------|------------|--------|-------|------|----------|--------|-------|------|
|                              | Mean        | Min.   | Max.   | SD    | CV   | Min.       | Max.   | SD    | CV   | Min.     | Max.   | SD    | CV   |
| Grain yield (kg/ha)          | 3735.6      | 2702.8 | 5116.6 | 801.0 | 21.4 | 3345.3     | 4206.0 | 378.1 | 10.1 | 3340.8   | 3983.2 | 236.1 | 6.3  |
| Test weight (kg/hl)          | 76.2        | 72.0   | 78.5   | 1.6   | 2.8  | 75.0       | 77.7   | 0.8   | 1.4  | 74.2     | 78.4   | 1.1   | 1.9  |
| Thousand kernel weight (g)   | 27.0        | 21.7   | 30.3   | 3.0   | 11.2 | 25.4       | 28.4   | 1.2   | 4.3  | 25.4     | 28.8   | 1.4   | 5.2  |
| Grain Protein (%)            | 13.2        | 10.3   | 16.6   | 1.8   | 13.9 | 12.2       | 14.2   | 0.9   | 6.6  | 12.5     | 13.7   | 0.6   | 4.2  |
| Flour yield (%)              | 70          | 70     | 70     | 0.0   | 3.2  | 70         | 70     | 0.0   | 0.4  | 70       | 70     | 0.0   | 1.7  |
| Flour ash (%)                | 0.5         | 0.5    | 0.6    | 0.0   | 5.9  | 0.5        | 0.5    | 0.0   | 1.5  | 0.5      | 0.5    | 0.0   | 2.3  |
| Flour protein (%)            | 11.8        | 9.0    | 15.3   | 1.8   | 15.6 | 10.9       | 12.8   | 0.8   | 7.2  | 11.2     | 12.3   | 0.5   | 4.2  |
| Falling Number (s)           | 476.7       | 441.6  | 530.8  | 30.3  | 6.4  | 466.1      | 483.4  | 7.2   | 1.5  | 465.4    | 485.6  | 7.6   | 1.6  |
| Water absorption (%)         | 58.6        | 56.5   | 64.4   | 2.7   | 4.6  | 57.6       | 59.7   | 0.8   | 1.4  | 57.2     | 59.7   | 0.8   | 1.4  |
| Dough Development Time (min) | 5.8         | 3.1    | 9.7    | 2.0   | 35.1 | 4.5        | 7.0    | 1.1   | 18.7 | 5.0      | 7.1    | 0.7   | 12.3 |
| Mixing tolerance index (BU)  | 28.6        | 19.6   | 48.1   | 9.6   | 33.8 | 26.0       | 31.8   | 2.2   | 7.7  | 18.7     | 37.1   | 5.9   | 20.8 |
| Dough stability (min)        | 11.4        | 6.1    | 13.8   | 2.7   | 23.8 | 10.2       | 12.6   | 1.2   | 10.3 | 9.4      | 14.3   | 1.7   | 15.1 |
| Loaf volume (mL)             | 2885.2      | 2771.9 | 2970.5 | 66.0  | 2.3  | 2871.5     | 2896.8 | 9.0   | 0.3  | 2817.2   | 2923.9 | 40.4  | 1.4  |

**Table 3.3. Percent variance components across the dataset for grain yield and the evaluated milling and baking functionality parameters as function of environment (E), genotype (G), management (M), and their interactions. GY – grain yield, TWT – test weight, TKW – thousand kernel weight, GP – grain protein, FY – flour yield, FA – flour ash, FP – flour protein, FNV – falling number value, WA – water absorption, DDT – dough development time, MTI – mixing tolerance index, -DS: dough stability, and LV – loaf Volume.**

| Component       | GY | TWT | TKW | GP | FY | FA | FP | FNV | WA | DDT | MTI | DS | LV |
|-----------------|----|-----|-----|----|----|----|----|-----|----|-----|-----|----|----|
| Environment (E) | 51 | 37  | 55  | 65 | 35 | 45 | 68 | 25  | 66 | 43  | 28  | 36 | 47 |
| Genotype (G)    | 4  | 17  | 11  | 6  | 11 | 8  | 5  | 1   | 6  | 4   | 11  | 15 | 19 |
| G x E           | 6  | 11  | 7   | 3  | 2  | 2  | 3  | 3   | 3  | 5   | 10  | 7  | 0  |
| Management (M)  | 12 | 11  | 8   | 16 | 0  | 3  | 16 | 1   | 7  | 14  | 0   | 7  | 0  |
| M x E           | 10 | 6   | 6   | 4  | 2  | 4  | 3  | 4   | 1  | 2   | 8   | 6  | 8  |
| G x M           | 1  | 2   | 1   | 0  | 0  | 0  | 0  | 0   | 0  | 1   | 0   | 0  | 0  |
| G x M x E       | 3  | 3   | 1   | 1  | 0  | 0  | 0  | 4   | 0  | 7   | 2   | 2  | 26 |
| Rep.            | 4  | 0   | 0   | 1  | 2  | 8  | 1  | 7   | 1  | 1   | 1   | 3  | -  |
| Residual        | 9  | 13  | 10  | 5  | 48 | 31 | 4  | 56  | 14 | 23  | 39  | 24 | 0  |

**Table 3.4. Linear regression coefficients ( $y = \alpha x + \beta$ ) and 95% confidence intervals of each trait on its respective environment mean for the different management intensities. The number of environments used in the calculation of the coefficients (degree of freedom, d.f., plus one) resulted from the combination of five genotypes and six Kansas environments. GY – grain yield, TWT – test weight, TKW – thousand kernel weight, GP – grain protein, FY – flour yield, FA – flour ash, FP – flour protein, FNV – falling number value, WA – water absorption, MTI, mixing tolerance index, DDT: dough development time DS – dough stability, and LV – loaf volume**

| Management   | Trait    | Yield       | TWT         | GP            | TKW           | FY          | FA          | FP            | FNV             | WA            | DDT         | MTI           | DS            | LV          |
|--------------|----------|-------------|-------------|---------------|---------------|-------------|-------------|---------------|-----------------|---------------|-------------|---------------|---------------|-------------|
| Standard     | d.f.     | 29          | 29          | 29            | 29            | 29          | 29          | 29            | 29              | 29            | 29          | 29            | 29            | 29          |
|              | $\alpha$ | 0.93        | 1.17        | 1.14          | 1.09          | 0.97        | 1.11        | 1.12          | 1.25            | 1.06          | 0.95        | 0.99          | 1.9           | 0.95        |
|              | CI       | (0.79-1.07) | (1.04-1.29) | (1.06-1.22)   | (0.99-1.18)   | (0.79-1.15) | (0.96-1.27) | (1.06-1.19)   | (1.07-1.44)     | (0.99-1.14)   | (0.77-1.13) | (0.82-1.15)   | (-0.98-4.79)  | (0.69-1.21) |
|              | $\beta$  | 3347        | 72.9        | 12.2          | 26.43         | 0.7         | 0.53        | 10.9          | 473.7           | 57.57         | 4.52        | 29.26         | 10.35         | 2885.57     |
|              | CI       | (3229-3466) | (72.6-73.2) | (12.05-12.36) | (26.12-26.75) | (0.69-0.7)  | (0.52-0.53) | (10.77-11.02) | (467.3-480.1)   | (57.35-57.78) | (4.1-4.93)  | (27.2-31.3)   | (8.93-11.77)  | (2865-2907) |
| High         | $r^2$    | 0.88        | 0.93        | 0.97          | 0.96          | 0.81        | 0.89        | 0.98          | 0.87            | 0.97          | 0.81        | 0.85          | 0.06          | 0.67        |
|              | $\alpha$ | 1.29        | 0.94        | 0.81          | 1.03          | 0.99        | 1.09        | 0.84          | 0.7             | 0.92          | 1.03        | 0.91          | 2.9           | 0.85        |
|              | CI       | (1.12-1.46) | (0.81-1.07) | (0.73-0.89)   | (0.9-1.16)    | (0.82-1.15) | (0.94-1.24) | (0.77-0.91)   | (0.38-1.02)     | (0.84-0.99)   | (0.87-1.19) | (0.72-1.09)   | (0.56-5.23)   | (0.59-1.1)  |
|              | $\beta$  | 4206        | 74.6        | 14.23         | 27.68         | 0.7         | 0.54        | 12.8          | 483             | 59.64         | 7.03        | 27.08         | 12.6          | 2887        |
|              | CI       | (4057-4354) | (74.3-74.9) | (14.07-14.38) | (27.23-28.13) | (0.69-0.7)  | (0.53-0.54) | (12.66-12.95) | (472.03-493.97) | (59.43-59.86) | (6.67-7.39) | (24.72-29.43) | (11.44-13.74) | (2866-2908) |
| High minus N | $r^2$    | 0.9         | 0.89        | 0.94          | 0.9           | 0.85        | 0.89        | 0.95          | 0.42            | 0.96          | 0.87        | 0.78          | 0.19          | 0.62        |
|              | $\alpha$ | 1           | 0.7         | 1.17          | 0.88          | 1.07        | 0.8         | 1.15          | 1.14            | 1.08          | 1.15        | 1.33          | 2.21          | 1.34        |
|              | CI       | (0.86-1.14) | (0.56-0.84) | (1.1-1.24)    | (0.75-1)      | (0.91-1.23) | (0.64-0.96) | (1.09-1.22)   | (0.88-1.41)     | (0.97-1.19)   | (1-1.3)     | (1.08-1.58)   | (-0.96-5.39)  | (1.12-1.54) |
|              | $\beta$  | 4006        | 75.3        | 12.4          | 28.38         | 0.69        | 0.52        | 11.09         | 465.34          | 57.92         | 4.95        | 31.66         | 10.3          | 2872.9      |
|              | CI       | (3883-4128) | (74.9-75.7) | (12.3-12.59)  | (27.93-28.82) | (0.69-0.7)  | (0.51-0.52) | (10.96-11.22) | (456.34-474.35) | (57.6-58.24)  | (4.61-5.29) | (28.54-34.77) | (8.7-11.8)    | (2856-2889) |
| High minus F | $r^2$    | 0.88        | 0.79        | 0.97          | 0.87          | 0.87        | 0.79        | 0.98          | 0.74            | 0.94          | 0.9         | 0.81          | 0.07          | 0.86        |
|              | $\alpha$ | 0.77        | 1.19        | 0.88          | 1             | 0.97        | 0.99        | 0.88          | 0.9             | 0.94          | 0.87        | 0.78          | 4.11          | 0.87        |
|              | CI       | (0.59-0.96) | (1.04-1.34) | (0.81-0.95)   | (0.85-1.16)   | (0.81-1.14) | (0.87-1.1)  | (0.82-0.94)   | (0.63-1.18)     | (0.86-1.02)   | (0.62-1.12) | (0.61-0.94)   | (1.59-6.64)   | (0.64-1.1)  |
|              | $\beta$  | 3385        | 72.7        | 13.86         | 25.4          | 0.7         | 0.54        | 12.54         | 484.39          | 59.11         | 6.78        | 25.7          | 12.8          | 2893.4      |
|              | CI       | (3223-3546) | (72.3-73.1) | (13.72-14)    | (24.87-25.96) | (0.69-0.7)  | (0.53-0.54) | (12.43-12.66) | (474.93-493.84) | (58.88-59.35) | (6.2-7.35)  | (23.6-27.8)   | (11.54-14.02) | (2875-2912) |
|              | $r^2$    | 0.72        | 0.9         | 0.96          | 0.86          | 0.84        | 0.92        | 0.97          | 0.61            | 0.95          | 0.65        | 0.77          | 0.28          | 0.68        |

**Table 3.5. Linear regression coefficients ( $y = \alpha x + \beta$ ) and 95% confidence intervals of each trait on its respective environment mean for the different genotypes. The number of environments used in the calculation of the coefficients (degree of freedom, d.f., plus one) resulted from the combination of five genotypes and six Kansas environments. GY – grain yield, TWT – test weight, TKW – thousand kernel weight, GP – grain protein, FY – flour yield, FA – flour ash, FP – flour protein, FNV – falling number value, WA – water absorption, MTI, mixing tolerance index, DDT: dough development time DS – dough stability, and LV – loaf volume**

| Genotype      | Trait    | Yield       | TWT         | GP            | TKW           | FY          | FA          | FP            | FNV             | WA            | DDT         | MTI           | DS            | LV          |
|---------------|----------|-------------|-------------|---------------|---------------|-------------|-------------|---------------|-----------------|---------------|-------------|---------------|---------------|-------------|
| WB4269        | d.f.     | 23          | 23          | 23            | 23            | 23          | 23          | 23            | 23              | 23            | 23          | 23            | 23            | 23          |
|               | $\alpha$ | 0.83        | 0.63        | 0.79          | 0.75          | 1.09        | 0.96        | 0.78          | 1.06            | 0.92          | 0.8         | 0.76          | 0.82          | 1.14        |
|               | CI       | (0.65-0.99) | (0.41-0.86) | (0.73-0.85)   | (0.6-0.91)    | (0.8-1.38)  | (0.83-1.08) | (0.73-0.84)   | (0.71-1.41)     | (0.82-1)      | (0.7-0.91)  | (0.51-1.02)   | (0.66-0.97)   | (0.91-1.37) |
|               | $\beta$  | 3983        | 74.7        | 12.5          | 26.7          | 0.68        | 0.52        | 11.23         | 485.56          | 59.05         | 5.05        | 27.08         | 10.67         | 2919.6      |
|               | CI       | (3822-4143) | (74.3-75.4) | (12.4-12.6)   | (26.17-27.2)  | (0.67-0.69) | (0.52-0.53) | (11.1-11.35)  | (473-56-497.56) | (58.79-59.31) | (4.78-5.3)  | (24.27-29.89) | (10.18-11.16) | (2903-2936) |
| WB4303        | $r^2$    | 0.82        | 0.6         | 0.97          | 0.82          | 0.74        | 0.92        | 0.97          | 0.64            | 0.95          | 0.91        | 0.64          | 0.84          | 0.83        |
|               | $\alpha$ | 0.97        | 0.72        | 0.99          | 0.77          | 0.88        | 0.88        | 0.99          | 0.89            | 1             | 1.19        | 1.47          | 1.39          | 0.83        |
|               | CI       | (0.81-1.13) | (0.58-0.86) | (0.91-1.1)    | (0.62-0.91)   | (0.72-1.04) | (0.68-1.1)  | (0.92-1.06)   | (0.62-1.16)     | (0.86-1.14)   | (0.92-1.46) | (1.24-1.71)   | (1.18-1.61)   | (0.58-1.08) |
|               | $\beta$  | 3688        | 72          | 13.6          | 28.4          | 0.69        | 0.54        | 12.22         | 471.73          | 59.69         | 6.21        | 28.54         | 12.57         | 2908        |
|               | CI       | (3540-3836) | (71.7-72.3) | (13.5-13.8)   | (27.91-28.88) | (0.68-0.7)  | (0.53-0.55) | (12.07-12.36) | (462.47-480.98) | (59.3-60.1)   | (5.57-6.86) | (25.97-31.12) | (11.89-13.25) | (2890-2926) |
| WB4458        | $r^2$    | 0.88        | 0.84        | 0.97          | 0.85          | 0.86        | 0.8         | 0.98          | 0.68            | 0.91          | 0.79        | 0.88          | 0.89          | 0.68        |
|               | $\alpha$ | 1.15        | 1.45        | 1             | 1.34          | 0.83        | 1.09        | 1.01          | 0.71            | 1.02          | 0.65        | 0.73          | 0.63          | 0.84        |
|               | CI       | (0.93-1.37) | (1.17-1.74) | (0.9-1.1)     | (1.2-1.49)    | (0.62-1.04) | (0.93-1.25) | (0.93-1.09)   | (0.36-1.07)     | (0.94-1.11)   | (0.52-0.78) | (0.37-1.1)    | (0.46-0.8)    | (0.45-1.22) |
|               | $\beta$  | 3328        | 73.2        | 13.7          | 28.7          | 0.69        | 0.54        | 12.24         | 479.45          | 58.68         | 5.51        | 37.08         | 9.39          | 2815.92     |
|               | CI       | (3126-3530) | (72.6-73.9) | (13.4-13.9)   | (28.25-29.21) | (0.68-0.7)  | (0.54-0.55) | (12.07-12.42) | (467.3-491.6)   | (58.44-58.93) | (5.19-5.82) | (33.07-41.08) | (8.85-9.94)   | (2788-2844) |
| WB4515        | $r^2$    | 0.84        | 0.84        | 0.95          | 0.94          | 0.75        | 0.9         | 0.97          | 0.44            | 0.96          | 0.82        | 0.44          | 0.75          | 0.48        |
|               | $\alpha$ | 0.99        | 1.05        | 1.18          | 1.01          | 1.18        | 1.03        | 1.17          | 1.31            | 0.95          | 1.37        | 0.81          | 1.14          | 1.24        |
|               | CI       | (0.89-1.11) | (0.94-1.16) | (1.11-1.25)   | (0.93-1.1)    | (0.95-1.41) | (0.85-1.22) | (1.12-1.23)   | (0.98-1.64)     | (0.78-1.12)   | (1.08-1.65) | (0.59-1.04)   | (0.91-1.38)   | (0.98-1.5)  |
|               | $\beta$  | 3707        | 76.1        | 13.6          | 25.4          | 0.71        | 0.51        | 12.26         | 463.67          | 57.15         | 7.02        | 18.69         | 14.33         | 2918.83     |
|               | CI       | (3608-3806) | (75.8-76.3) | (13.49-13.78) | (25.14-25.72) | (0.71-0.72) | (0.5-0.52)  | (12.14-12.37) | (452.49-474.84) | (56.67-57.64) | (6.34-7.71) | (16.2-21.18)  | (13.6-15.07)  | (2899-2937) |
| WB-Grainfield | $r^2$    | 0.94        | 0.95        | 0.98          | 0.96          | 0.84        | 0.86        | 0.99          | 0.76            | 0.86          | 0.82        | 0.72          | 0.83          | 0.82        |
|               | $\alpha$ | 1.06        | 1.14        | 1.04          | 0.75          | 1.01        | 1.05        | 1.04          | 1.03            | 1.12          | 1           | 1.22          | 1.01          | 0.95        |
|               | CI       | (0.93-1.19) | (1.03-1.25) | (0.96-1.13)   | (0.56-0.91)   | (0.81-1.22) | (0.88-1.21) | (0.96-1.11)   | (0.84-1.22)     | (1.03-1.2)    | (0.86-1.13) | (1-1.44)      | (0.88-1.15)   | (0.7-1.21)  |
|               | $\beta$  | 3972        | 73.3        | 12.5          | 26.7          | 0.71        | 0.53        | 11.22         | 482.62          | 58.23         | 5.31        | 30.74         | 10.5          | 2861.79     |
|               | CI       | (3847-4097) | (73-73.6)   | (12.4-12.7)   | (26.17-27.2)  | (0.7-0.71)  | (0.52-0.53) | (11.06-11.38) | (475.98-489.27) | (57.99-58.47) | (4.99-5.63) | (28.33-33.15) | (10.08-10.93) | (2843-2881) |
|               | $r^2$    | 0.93        | 0.95        | 0.97          | 0.82          | 0.83        | 0.89        | 0.97          | 0.85            | 0.97          | 0.92        | 0.86          | 0.92          | 0.73        |

## Figures

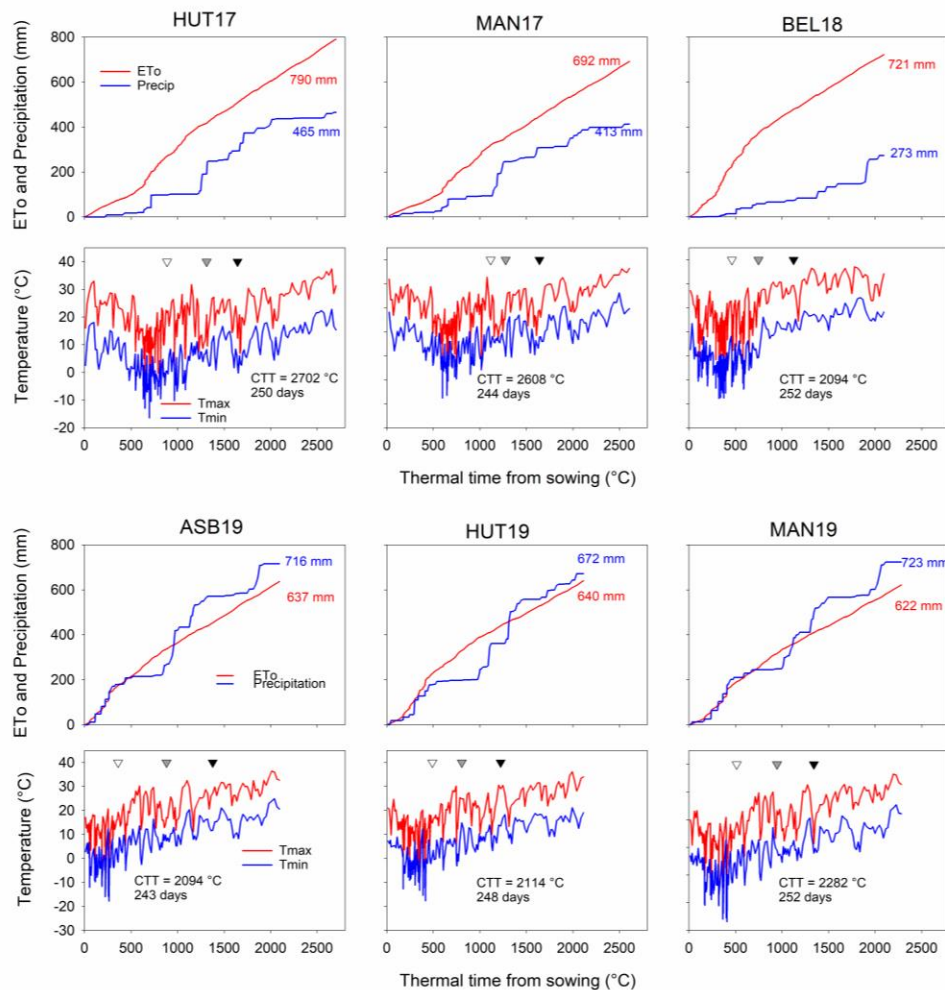


**Figure 3.1. Cumulative reference evapotranspiration (ETo) and precipitation (first and third rows), and minimum and maximum temperatures (second and fourth rows) during the winter wheat growing season in six Kansas environments (ASH, Ashland Bottoms; BEL, Belleville; HUT, Hutchinson; MAN, Manhattan; 17, 2016-17 growing season; 18, 2017-18 growing season; 19, 2018-19 growing season). Downward-facing triangles show application dates for fertilizers (Feekes 4), early fungicide (Feekes 6), and late fungicide (Feekes 10.5). Inset values show cumulative ETo, precipitation, cumulative thermal time (CTT), and growing season duration.**

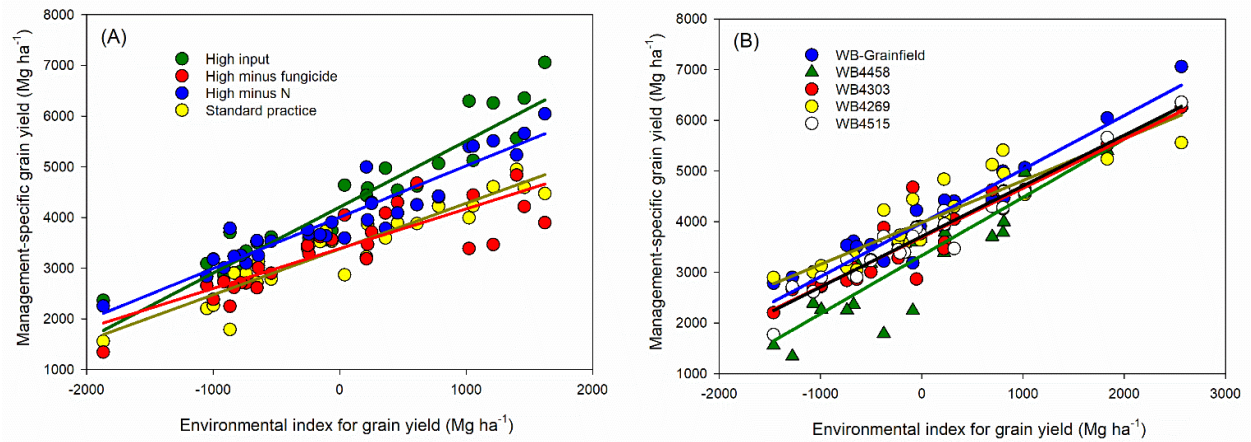


**Figure 3.2. Stability analysis through linear regression of grain yield as impacted by environmental index for grain yield for the (A) management × environment interaction and the (B) genotype by environment interaction. Coefficients of the regression and 95% confidence intervals are shown in Tables 4 and 5.**

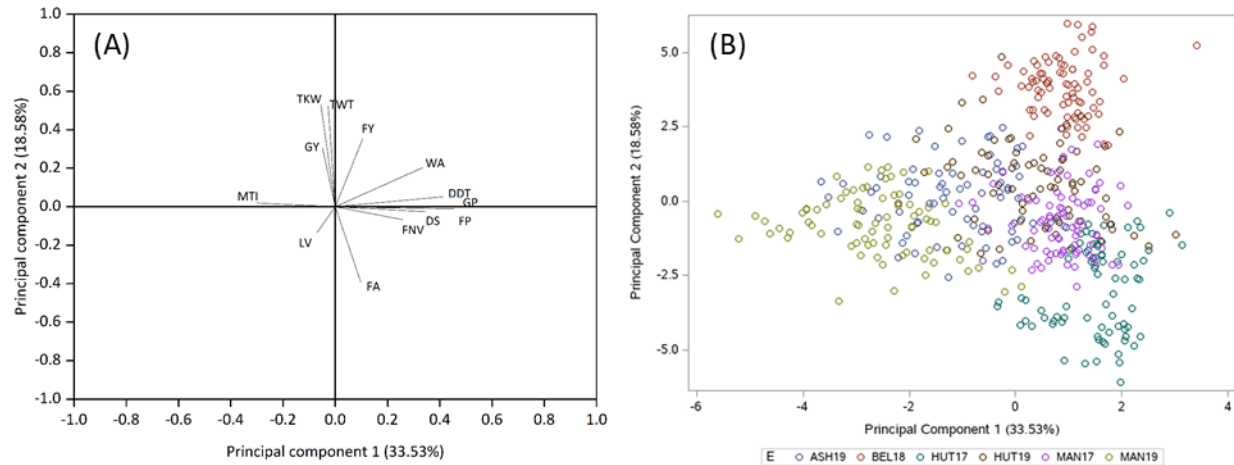


**Figure 3.3. (A) Pattern plot for the examined traits and values of PC1 and PC2 for the experimental combination of environments, genotype, and management practices (GY – grain yield, TWT – test weight, TKW – thousand kernel weight, GP – grain protein, FY – flour yield, FA – flour ash, FP – flour protein, FNV – falling number value, WA – water absorption, DDT – dough development time, DS – dough stability, MTI – mixing tolerance index, and LV – loaf volume), and (B) biplot of the traits grouped based on environments (ASH, Ashland Bottoms; BEL, Belleville; HUT, Hutchinson; MAN, Manhattan; 17, 2016-17 growing season; 18, 2017-18 growing season; 19, 2018-19 growing season).**

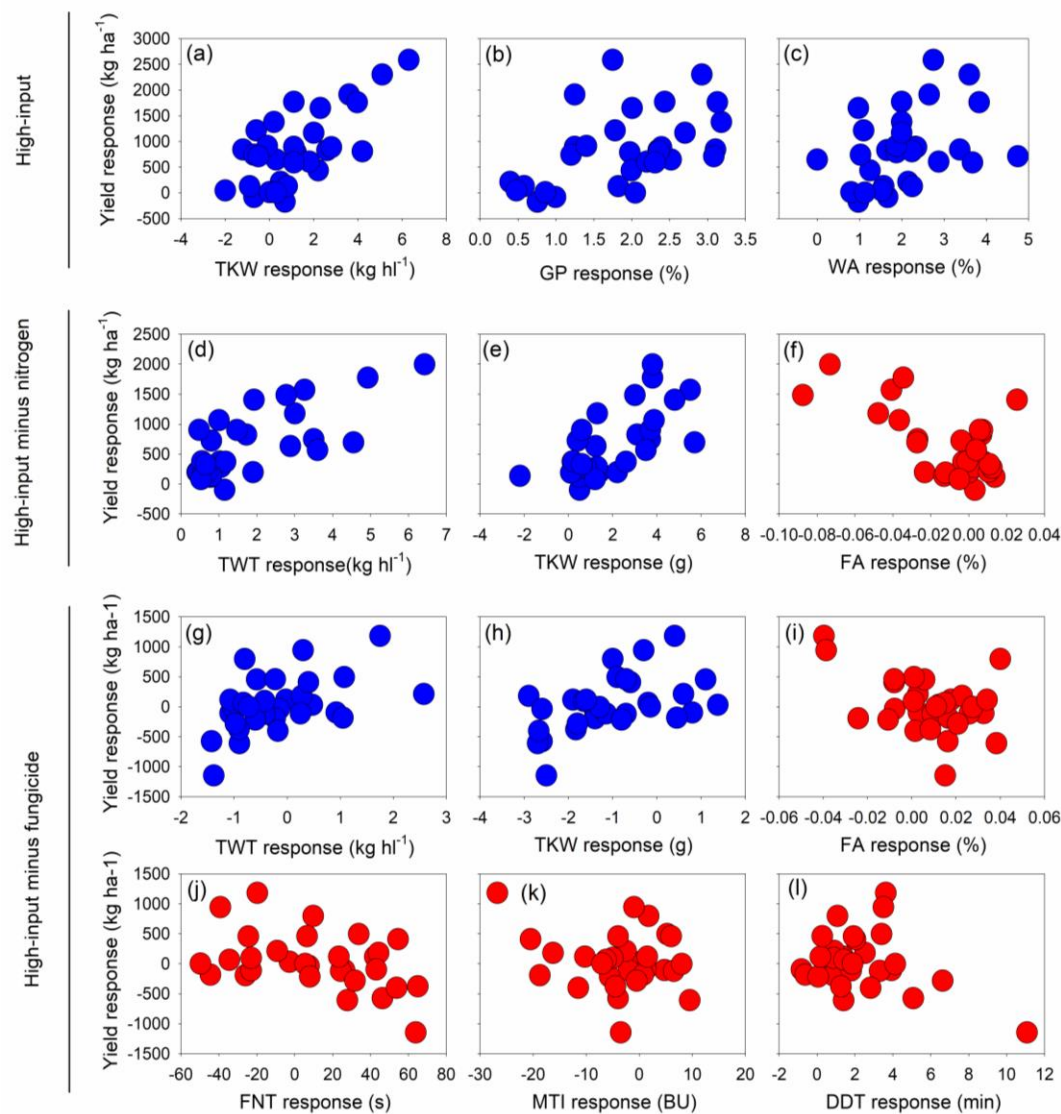


**Figure 3.4. Scatter matrix of relationships between the response of grain yield (dependent variable) and the response of different grain, mill, and bake quality parameters (independent variables) to high-input management (a-c), high-input minus nitrogen (d-f), and high-input minus fungicide (g-l) for five genotypes grown in six Kansas environments. Blue markers indicate significant positive and red markers indicate significant negative association between variables.**

## **Chapter 4 – Moisture diffusion modelling of wheat kernels during tempering**

### **Abstract**

The study investigated moisture movement within the kernel during tempering. The moisture diffusion coefficient ( $1.63 - 3.81 \times 10^{-11} \text{ m}^2/\text{s}$ ) was determined using experimental absorption data. Subsequently, finite element analysis (FEA) was employed to model the moisture distribution within the kernel. This model predicted that the core of the kernel reached the desired tempering moisture content within 12 h. The predicted moisture distribution was then validated using magnetic resonance imaging (MRI) analysis. This combined approach offers a valuable tool for predicting moisture absorption dynamics during tempering. Such predictions can be used to tailor tempering regimes for optimal outcomes in wheat milling.

### **4.1 Introduction**

Tempering is the process of conditioning wheat that increases milling efficiency. The process comprises adding a calculated amount of water to the wheat followed by a resting stage. This ensures the migration of water to wheat. The process toughens the bran and germ whereas it mellows the endosperm. Softening of the endosperm allows it to be reduced without creating excess of damaged starch (Cappelli et al., 2020). Addition of water to the wheat kernels causes plasticization of the biopolymers (polysaccharides and proteins). Water molecules weaken the dipole-dipole interactions and interferes with the intra and inter molecular hydrogen bonds between these biopolymers. This lowers the fracture strength and elastic modulus of the bran tissues resulting in extensibility (Hemery et al., 2010). This helps to recover bran as large particles and help in effective separation.

Several factors including, temperature, kernel characteristics, wheat variety, and tempering time are known to affect the moisture migration inside the wheat kernel (Kang & Delwiche, 2000). Studies have shown that increasing tempering moisture can decrease flour yield (Hourston et al., 2017) and increase energy consumption (Warechowska et al., 2016). However, lower tempering moisture results in higher bran content and decreased baking quality of the flour (Cappelli et al., 2020). This highlights the need for a balance between tempering process and flour extraction. Furthermore, shorter tempering durations may not ensure complete water diffusion, while longer durations can significantly increase microbial load (Lin et al., 2023). Currently, the standard tempering process reportedly exceeds 18 h (18 – 24 h for soft wheat and 24 – 30 h for hard wheat), potentially impacting the microbial safety of wheat and wheat flour (Liu et al., 2023). Therefore, a deeper understanding of moisture distribution and movement within the wheat kernel could lead to improved control of the tempering process, optimizing both flour quality and microbial safety.

Moisture migration during grain processing has been subject to investigation, particularly soaking (Dutta et al., 2020; Kang & Delwiche, 1999; Shorstkii et al., 2022). However, research on moisture movement within the wheat kernels specifically during the tempering is scarce (Hsu, 1984). Existing models for moisture diffusion often simplify the kernel geometry, representing it as a sphere (Igathinathane & Chattopadhyay, 1997) or infinite cylinder (Muthukumarappan & Gunasekaran, 1990). Additionally, these models frequently treat the kernel as a homogeneous material, neglecting its internal structural variations. While (Muthukumarappan & Gunasekaran, 1990) explored the influence of geometry on corn kernel diffusion coefficients, (Kang & Delwiche, 2000) further evaluated the impact of geometry and endosperm and pericarp

diffusivity using numerical methods. It is important to note that these prior studies focused on moisture migration during soaking, not tempering.

This study addresses this gap in knowledge by analyzing moisture migration during the tempering process using finite element modeling (FEM). We hypothesized that a higher final tempering moisture content would reduce the required tempering time due to faster and more uniform moisture diffusion within the kernel. To achieve this, we developed a finite element model (FEM) as the first stage of our research. This initial model considered a homogeneous wheat kernel tempered to 16% moisture content and analyzed the resulting moisture migration pattern. This analysis provided a foundation for further exploration of how varying final moisture content and incorporating the kernel's complex internal structure would influence moisture diffusion and ultimately, tempering efficiency.

## **4.2 Materials and Methods**

### **4.2.1 Materials and sample preparation**

Hard red winter (HRW) wheat samples obtained from Montana Flour and Grains (Fort Benton, Montana, USA) were selected for the study. The moisture content of the sample was determined following the standard procedure ASABE Method S352.2 (ASAE S352.2, 2009). Briefly, 10g of wheat kernels were dried in the oven at 130 °C for 19h. After drying, the samples were weighed to record the final weight. The change in weight over the period is associated with the loss of unbound moisture. Thus, the moisture content of the samples was calculated as equation 4.1

$$C_{mass} = \frac{M_w}{M_D + M_w}$$

Where,  $M_w$  is the mass of water and  $M_D$  is the mass of dry material of wheat kernel.

The true density of the kernels was measured using a gas pycnometer (Ultracyc 1200e, Quantachrome Instruments, USA). The pycnometer used gas (helium) displacement technique to determine the volume of known quantity of wheat. Further from the mass and volume, the true density of the sample was calculated.

Geometric properties of individual wheat kernels were measured using digital caliper (UltraTech, General Tools & Instruments, USA). Three principal axes of 20 randomly selected kernels (i.e., L: length, W: width and T: thickness) were measured. Equivalent diameter ( $D_p$ , Eq. 4.2), geometric diameter ( $D_g$ , Eq. 4.3) and sphericity ( $\phi$ , Eq. 4.4) of the wheat kernels was calculated as per equation (Escalante-Aburto et al., 2023). The properties of the HRW samples selected for the study are detailed in Table 4.1.

$$D_p = \left( \frac{L \times (W + T)^2}{4} \right)^{1/3}$$

$$D_g = (LWT)^{1/3}$$

$$\phi = \frac{D_g}{L}$$

Moisture content of the samples was adjusted to 16% wet basis, (0.19 g of water/g of solids) following the standard procedure outlined in AACC 26-10.02 (AACC, 2009). The amount of water to be added was calculated according to the following equation (Eq. 4.5).

*Water added (ml)*

$$= \frac{\text{Mass of wheat} \times (\text{Final target moisture} - \text{Initial moisture content})}{(100 - \text{Final target moisture})}$$

Water was added to the measured quantity of wheat kernels (100g) to increase their moisture content to 16%. Following through mixing, the kernels were sealed in polyethylene bags and placed in the storage chamber (Model I-36 VL, Pervical Scientific Inc., Iowa, USA). The samples were kept at a consistent temperature of  $22.0 \pm 0.5$  °C, and the storage chamber maintained an equilibrium relative humidity corresponding to the desired moisture content.

## 4.2.2 Development of mathematical model

### 4.2.2.1 Theoretical background

Wheat is a hygroscopic capillary porous material (Ghosh et al., 2008). During the tempering process moisture is transferred from the surface of the kernel to its interior by diffusion.

Moreover, the process occurs at constant temperature and pressure. Thus, the diffusion process follows Fick's second law. The governing equation (Eq. 4.6) for this diffusion process is as follows:

$$\frac{\partial C}{\partial t} = D \left( \frac{\partial^2 m}{\partial r^2} + \frac{\partial m}{r \partial r} + \frac{\partial^2 m}{\partial z^2} \right)$$

Where

D = diffusion coefficient (m<sup>2</sup>/s)

C = moisture concentration (g of water/ g of solid)

r = radial coordinate (m)

z = axial coordinate (m)

t = time (s)

For the migration study, the following assumptions were considered: (1) the wheat kernel is isothermal and heat transfer is neglected; (2) kernel volume change is negligible during the tempering process; (3) the endosperm and pericarp are homogenous.

The boundary and initial conditions applied for the study were: (1) the initial moisture content is distributed uniformly within the wheat kernel ( $m_{in}$ ); (2) at time  $t = 0$ , the surface moisture content of the kernel is in equilibrium with the environment ( $m_{eq}$ ).

The finite element analysis (FEA) was used to theoretically solve the system of moisture transfer equations in a cartesian coordinate system. The governing equations underwent transformation into element equations through the following steps:

Considering the diffusion equation in its differential form (Eq. 4.7):

$$\frac{\partial C}{\partial t} = D \nabla \cdot (\nabla C)$$

The concentration inside each element was determined using linear interpolation. In this case, the concentration field,  $C$  and the weight function ( $v$ ) are calculated using the interpolation function,  $N_A, N_B, N_C$  (Eq. 4.8 – 4.12):

$$C \approx C_A N_A + C_B N_B + C_C N_C$$

$$v \approx v_A N_A + v_B N_B + v_C N_C$$

$$\text{Where, } N_A(\xi, \eta) = 1 - \xi - \eta$$

$$N_B(\xi, \eta) = \xi$$

$$N_C(\xi, \eta) = \eta$$

Here,  $\xi$  and  $\eta$  are the barycentric coordinates that vary from 0 to 1 within the triangular element.

Multiplying the differential equation by weight function ( $v$ ) and integrating over the volume ( $\Omega$ ), the weak form integral of the Laplacian term was obtained as (Eq. 4.13)

$$\int_{\Omega} \frac{\partial C}{\partial t} v d\Omega = D \int_{\Omega} \nabla \cdot (\nabla C) v d\Omega$$

Then, Gauss's divergence theorem was applied to transform the volume integral into a surface integral (Eq. 4.14),

$$\int_{\Omega} \frac{\partial C}{\partial t} v d\Omega = D \int_{\partial\Omega} \nabla C \cdot \mathbf{n} v d\mathbf{S} - D \int_{\Omega} \nabla C \cdot \nabla v d\Omega$$

Where  $\partial\Omega$  represents the boundary of the domain,  $\mathbf{n}$  is the outward normal vector, and  $d\mathbf{S}$  denotes the differential surface element.

Furthermore, Dirichlet boundary conditions were chosen to incorporate the boundary conditions necessary for calculating the concentration.

Finally, after discretizing time, all the individual equations for each finite element were combined to obtain the system of equations in the form (Eq. 4.15)

$$M \frac{dC}{dt} = KC$$

Where,  $M$  is the mass matrix,  $K$  is the stiffness matrix, and  $C$  represents the vector of concentrations at the nodes of the element.

Assuming the density of the kernel as  $1260 \text{ kg/m}^3$  and porosity as 5%, the mass average method was used to determine moisture distribution of the kernel.

#### 4.2.2.2 Finite element modelling

The time dependent moisture distribution inside the kernel was determined using MATLAB (R2023b, MathWorks, USA). The MATLAB partial differential equation (PDE) toolbox played a pivotal role in simplifying the analysis by providing built-in functions for mesh generation, PDE solving and post processing. In the study of intact kernel, one quarter of an ellipse was used in time dependent axisymmetric two-dimensional analysis. Subsequently, a triangular mesh was generated with maximum element size of 0.1. Following this, the PDE model was created, and the diffusion coefficient was specified. By assuming uniform distribution of the initial moisture content (0.085 g of water/ g of solids) within the kernel, and equilibrium moisture content of 0.19 g of water/ g of solids, the system of equations was solved to calculate the moisture distribution.

#### **4.2.3 Magnetic resonance imaging (MRI)**

Moisture distribution within the wheat kernels following tempering was assessed through magnetic resonance imaging (MRI) experiments. The experiments utilized a 14.1 T (600 MHz) MRI instrument (Ascend 600 WB, Bruker Co., USA). Wheat kernels were tempered for varying tempering durations (6, 12, 18, and 24 h) for the MRI analysis. Control samples comprised both untampered wheat kernels and kernels soaked for varying durations (2h and 4h). The kernels were packed into NMR tubes (5 mm outer diameter). These NMR tubes, containing both tempered and soaked kernels along with control samples, were arranged in a custom-built sample holder inserted into the probe. Before the experiments, soaked kernels were blotted to remove excess water from its surface.

For MRI analysis, a two-dimensional multi-slice spin echo pulse sequence was used. The parameters used for MRI analysis are reported in Table 4.2. All the images were taken in transverse slices

## **4.3 Result and discussion**

### **4.3.1 Moisture diffusion**

The effective diffusivity of wheat kernels ranged from  $1.63 - 3.81 \times 10^{-11} \text{ m}^2/\text{s}$  (table 4.3). For example, when the kernels were tempered to 16% (wet basis, equal to 0.19 g of water/ g of solids), the effective moisture diffusivity was  $2.45 \times 10^{-11} \text{ m}^2/\text{s}$ , whereas it increased to  $3.81 \times 10^{-11} \text{ m}^2/\text{s}$  with a tempering moisture content of 18% (wet basis). Although there was a variability in diffusivity with moisture content, these changes were not statistically significant ( $p > 0.05$ ). Notably, there are wide disparities in moisture diffusivities reported in the literature (Igathinathane & Chattopadhyay, 1997; Kang & Delwiche, 2000; Xingjun & Ping, 2016). These differences may be attributed to variations in the studied varieties and experimental conditions. With few exceptions, such as studies by (Xingjun & Ping, 2016), the reported diffusivities were derived from soaking studies where moisture availability is unrestricted for migration. This unrestricted moisture availability during soaking leads to volume expansion of the kernels, consequently increasing the diffusivity, as highlighted by (Bello et al., 2010; Dutta et al., 2020).

### **4.3.2 Finite element modelling**

It is important to note that in the FEM analysis, the wheat kernels are treated as prolate spheroid. To accommodate this non-spherical geometry, a correction method outlined by Kang and Delwiche (Kang & Delwiche, 2000) is employed. The corrected diffusivities are reported in Table 4.3. Specifically, for FEM analysis, the diffusivities corresponding to the non-spherical geometry correction were utilized.

Figure 4.1 (a) and (b) illustrate the time dependent moisture diffusion within soaked wheat kernels. After 2 h and 4 h of soaking, the moisture content at the kernel's core increased to 0.2 g

of water/ g of solids and 0.35 g of water/ g of solids, respectively. Figure 4.2 shows the time dependent moisture distribution inside the kernels following tempering process. As described in the previous section, the initial moisture content of the wheat kernel was 0.085 g of water/ g of solids, and was assumed to be uniformly distributed inside the kernels. On tempering, the moisture on the surface is increased to 0.19 g of water/ g of solids (Figure 4.2a). Over time, the moisture distributes inside the kernel. For instance, the moisture content at core of the kernel increased to 0.11 g of water/ g of solids by 6h of tempering (Figure 4.2b). Figure 4.2c illustrates the moisture distribution following 12h of tempering. Consequently, after 12h, the moisture content at the center of the kernel is 0.18 g of water/ g of solids, indicating moisture penetration towards the core.

#### **4.3.3 MRI analysis**

The MRI images in figure 4.3 represent the moisture distribution within wheat kernels subjected to varying durations of tempering. Brighter regions in the images signify higher moisture, as reported by (Hu et al., 2019). The analysis reveals a nonuniform distribution of moisture within the kernels, with regions near the epidermis (seed coat) exhibiting greater moisture content compared to the endosperm regions. However, the internal moisture distribution within the kernel was not readily apparent from the figure. Furthermore, figure 4.4 illustrates the moisture movement within soaked wheat kernels. Following 2h of soaking, the moisture content reached 0.283 g of water/ g of solids, increasing to 0.4263 g of water/ g of solids after 4h. This substantial increase in moisture content compared to tempered kernels is evident in the MR images, with soaked kernels having brighter regions indicative of heightened moisture content. The results indicate a directional flow of moisture during the tempering process, with moisture migrating from the outer layers towards the endosperm. The brightness of the observed MR

image directly corresponds to the moisture distribution within the kernels. However, it is noteworthy that in the studies, the examined kernels had a moisture of 0.19 g of water/ g of solids, which constrained the intensity of the MR images. To obtain MR images with a higher signal to noise ratio, it is imperative that the moisture content of the kernels reaches at least 0.25 g of water/ g of solids, as recommended by (Ghosh et al., 2007). Furthermore, during the initial hours of moisture absorption, there is a rapid increase in the percentage of bound water; while the increment in free water is comparatively slower, as documented by (Ying et al., 2020). Moreover, in heterogeneous systems such as grains, variations in water content among starch granules, cell walls, and pericarp result in differing relaxation times, as outlined by (Ghosh et al., 2008; Ying et al., 2020). These inherent variabilities contribute to differences in the MR intensity observed in the images.

#### **4.4 Conclusion**

This study successfully determined the moisture diffusion coefficient of wheat kernels through absorption experiments. Using this data, finite element analysis (FEA) effectively modeled the moisture distribution within the wheat kernel during tempering. The model indicated that the core reaches the desired tempering moisture content within 12 hours. Magnetic resonance image (MRI) analysis provided qualitative validation of the moisture distribution predicted by FEA. However, further studies are warranted to develop quantitative methods for moisture distribution analysis.

These combined approaches enable the prediction of moisture absorption dynamics during tempering facilitating the tailoring of tempering regimes for optimal outcomes. However, it is important to acknowledge that the FEA model simplified the wheat kernel by treating it as a homogenous entity. This approach overlooks the inherent heterogeneity of the kernel, which

consists of distinct components with varying diffusion characteristics such as endosperm, pericarp, and germ. Future models should aim to incorporate these complexities for more accurate predictions of moisture migration. Furthermore, exploring three-dimensional analysis of the moisture migration with porous modelling could provide deeper insights into the intricate dynamics of tempering.

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## Tables

**Table 4.1. Properties of un-tempered HRW (control) samples**

| Properties                                 |                   | Hard Red Winter<br>(HRW) |
|--------------------------------------------|-------------------|--------------------------|
| Kernel dimensions:                         | Length (L), mm    | 6.16 (0.3)               |
|                                            | Width (W), mm     | 2.91 (0.1)               |
|                                            | Thickness (T), mm | 2.67 (0.1)               |
| Equivalent diameter ( $D_p$ ), mm          |                   | 3.63 (0.08)              |
| Geometric diameter ( $D_g$ ), mm           |                   | 3.63 (0.08)              |
| Sphericity                                 |                   | 0.59 (0.02)              |
| Moisture content (% , wet basis)           |                   | 8.58 (0.11)              |
| Moisture content (g of water/ g of solids) |                   | 0.09                     |
| Protein content* (% , 14% moisture basis)  |                   | 10.19 (0.05)             |
| True density*, $\text{kg/m}^3$             |                   | 1260.1 (2.1)             |

Measurements are reported as mean (standard deviation), representing an average of 20 readings. \*Measurements are average of 3 readings

**Table 4.2. Parameters used in MRI instruments**

| <b>Parameter</b>       | <b>Value/ description</b>             |
|------------------------|---------------------------------------|
| Repetition time (TR)   | 31.398 ms                             |
| Echo time (TE)         | 1.4 ms                                |
| Flip angle             | 80                                    |
| Number of slices       | 8                                     |
| Slice thickness        | 0.5 mm                                |
| Field of view (FOV)    | 30 mm × 30 mm                         |
| Image resolution       | 117 $\mu\text{m}$ × 117 $\mu\text{m}$ |
| Image acquisition time | 2 min 40 s 755 ms                     |
| Number of averages     | 32                                    |

**Table 4.3. Effective diffusivity with tempering**

| <b>Moisture<br/>(%, wet basis)</b> | <b>Effective diffusivity (<math>D_{\text{eff}}</math>, <math>10^{-11} \text{ m}^2 \text{ s}^{-1}</math>)</b> |                                                                                          |
|------------------------------------|--------------------------------------------------------------------------------------------------------------|------------------------------------------------------------------------------------------|
|                                    | <b><math>D_{\text{eff}}</math></b>                                                                           | <b>Non-spherical geometry<br/>correction (<math>D_{\text{eff}} \times \phi^2</math>)</b> |
| 14                                 | 1.63 (0.8) <sup>A</sup>                                                                                      | 0.57 (0.4) <sup>A</sup>                                                                  |
| 16                                 | 2.45 (0.9) <sup>A</sup>                                                                                      | 0.85 (0.5) <sup>A</sup>                                                                  |
| 18                                 | 3.81 (0.4) <sup>A</sup>                                                                                      | 1.33 (0.4) <sup>A</sup>                                                                  |

Measurements are reported as mean (standard deviation), representing the average of 3 readings. Values with the same case letters within a column are not statistically different ( $\alpha = 0.05$ ).

## Figures

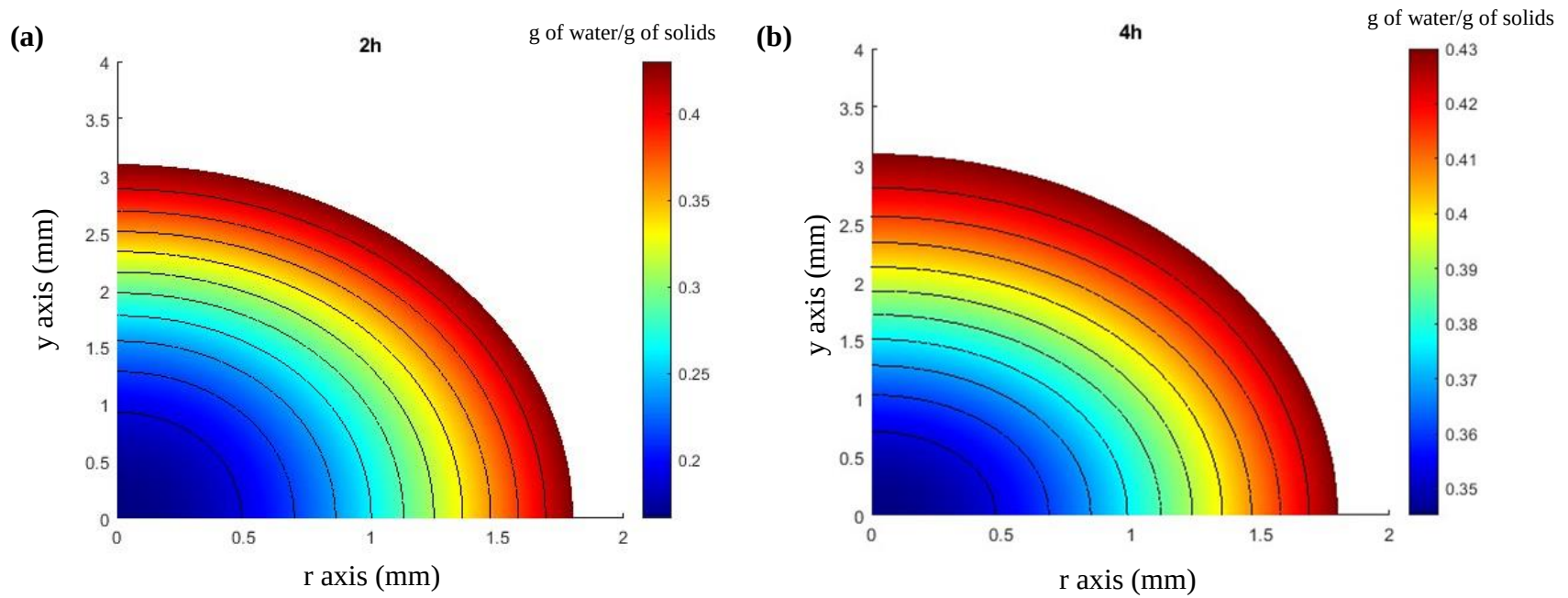


**Figure 4.1.** Typical distribution of moisture in a soaked wheat kernel determined by finite element analysis (a) 2h (b)4h

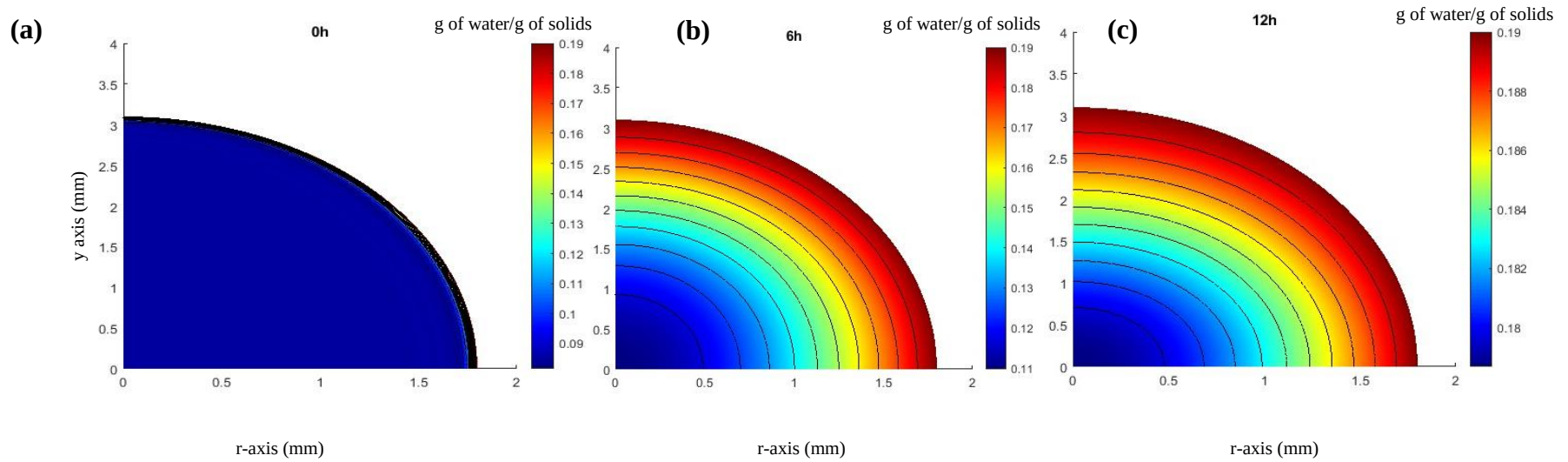


**Figure 4.2. Typical distribution of moisture in a tempered wheat kernel determined by finite element analysis (a) 0h (b)6h (c) 12h**

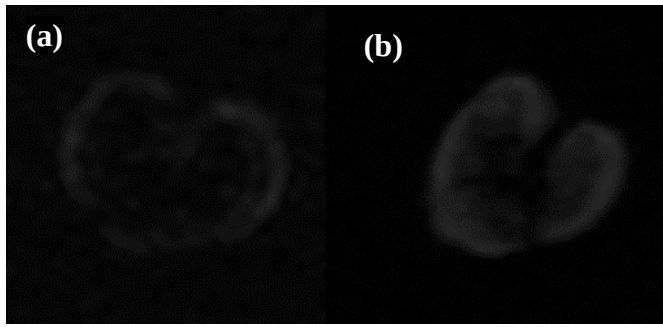


**Figure 4.3.** Two-dimensional magnetic resonance (MR) image of wheat kernel following tempering (a) 6h (b)12 h. Bright regions indicate higher water concentration.

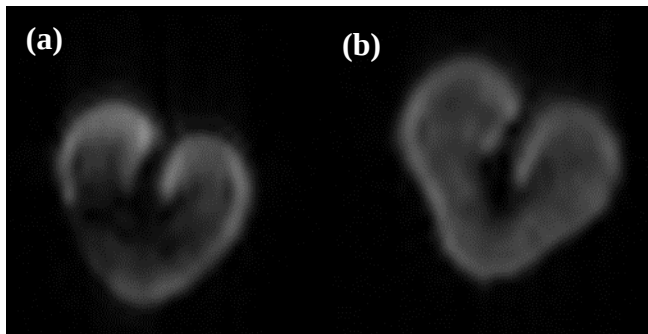


**Figure 4.4.** Two-dimensional magnetic resonance (MR) image of wheat kernel following soaking (a) 2h (b) 4 h. Bright regions indicate higher water concentration.

## **Chapter 5 – Time dependent changes in the compression behavior of single wheat kernels upon tempering<sup>2</sup>**

### **Abstract**

Tempering, the controlled addition of water to wheat prior milling, is a crucial step in improving the efficiency of flour extraction. However, the limited availability of water significantly impacts moisture migration within the kernels, consequently influencing their breakage behavior. This study delves into the effects of tempering time (3, 6, 9, and 12 h) and moisture content (14%, 16% and 18%) on the moisture diffusivity and compressibility characteristics of single wheat kernels from hard red winter (HRW) and hard red spring (HRS) varieties. Uniaxial compression tests revealed a significant influence of tempering time on the viscoelastic properties of the kernels. The elastic modulus of HRW kernels varied from 89.2 to 155.8 MPa, while that of HRS kernels ranged from 115.0 to 192.2 MPa. Kernel diffusivity exhibited variations with tempering moisture, although these differences were not statistically significant ( $p > 0.05$ ). Elastic work decreased from 8.8 to 5.4 N.mm, whereas plastic work increased to 1.9 N. mm upon increasing the tempering moisture content. Notably, the changes in compressibility follow first order kinetics at all moisture levels. The rate constant for compressibility ranged from 0.002 to 0.0057  $\text{h}^{-1}$  for HRS and from 0.0026 to 0.0066  $\text{h}^{-1}$  for HRW, respectively. These findings provide insights into the interaction between tempering conditions and kernel properties, enabling the optimization of tempering processes for improved efficiency.

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## 5.1 Introduction

Wheat (*Triticum aestivum*) occupies a prominent position as a globally utilized grain, with an annual production of 770.88 million metric tons (FAOSTAT, 2023). Its versatility extends across diverse applications with food comprising the most significant share (66%), followed by feed and other industrial purposes (21%) and propagation material (10%) (Erenstein et al., 2022; Psaroudaki, 2007). Unlike rice, typically consumed as whole kernels (Siaw et al., 2021) wheat requires size reduction for consumption, resulting in semolina or flour. Wheat milling is a multi-stage grinding process that transforms wheat kernels into flour (Dziki, 2011). The quality of the resulting flour depends on the properties of wheat (Acar et al., 2019), design of the milling machinery and the operating conditions (Baasandorj et al., 2015). Since the milling process significantly influence the end use quality of the flour, proper management of this unit operation is crucial (Cappelli & Cini, 2021).

One of the critical steps in the milling process is tempering or conditioning, which involves increasing the moisture content of the wheat kernels to a level suitable for milling, depending on the wheat type. The process is essential for creating friability differences between the bran and endosperm (Cappelli et al., 2020) It softens the endosperm and toughens the bran, facilitating the separation of these components during the milling process. For hard wheat varieties, a tempering moisture content of 16 - 16.5% is considered optimum for milling whereas for soft wheat, a range of 14 -14.5% is generally recommended.

Detailed insights into water uptake, moisture migration and diffusion during the tempering process have been provided by studies conducted by (Kang & Delwiche, 1999) and (Delwiche, 2000). According to El-Porai and co-authors (El-Porai et al., 2013) it is essential to allow sufficient time for water to penetrate the core of the kernels during tempering. Inadequate

tempering can result in reduced bran friability and increased fragility of the starch rich endosperm (Pagani et al., 2014). The tempering moisture content, temperature, time and kernel properties (wheat type, initial moisture content, protein content) reportedly influence the rate of moisture uptake by the kernels (Abo-Dief et al., 2019; El-Porai et al., 2013). Researchers have extensively explored the impact of tempering process on milling quality, flour characteristics (Cappelli et al., 2020; Kweon et al., 2009) and energy requirements (Warechowska et al., 2016). While the effect of tempering on these aspects are well established, understanding the influence on the individual kernel characteristics is crucial to advance the studies in modelling the milling process.

Throughout the milling, the wheat kernels are subjected to various forms of loading. Thus, comprehending the mechanics of wheat crushing or cracking is a prerequisite for determining the work involved in the process and subsequently calculating energy requirements. Compression tests offer insights into the peak force a grain can withstand, essentially assessing the force required to induce deformation through compression. The uniaxial compression characteristics of grain kernels are influenced by factors such as moisture content, temperature, and loading rate (Nwakuba et al., 2022; Zareiforush et al., 2012). Investigations into grain mechanical properties are conducted on either individual kernels or in bulk (Su et al., 2019). Crucially, the loading pattern differs significantly when studying individual kernels compared to bulk samples (Foutz et al., 1993).

Numerous researchers have investigated moisture-dependent alterations in the mechanical properties of wheat kernels. In studies conducted by Haddad et al., (Haddad et al., 2001) and Delwiche (Delwiche, 2000) intact wheat kernels were transformed into regular cylinders to facilitate the evaluation mechanical properties. However, these modifications may potentially

impact the kernel's properties due to the formation of minor cracks during machining.

Compression characteristics of intact wheat kernels tempered to different moisture contents were reported by several authors (Escalante-Aburto et al., 2023; Figueroa et al., 2011; Ponce-García et al., 2008, 2013). Moreover, tempering induced changes in the mechanical properties have an impact on rupture force and grinding energy during milling. Previous studies have specifically investigated the influence of tempering moisture on grinding energy (Dziki, 2011; Fang & Campbell, 2003; Warechowska, 2014; Warechowska et al., 2016). In all these studies, the wheat kernels were conditioned for a minimum of 24h at the specified moisture content before the experiments to ensure migration of moisture to the kernel's interior.

Nevertheless, the mechanical behavior of food grains is time-dependent, as indicated by Bargale et al. (Bargale et al., 1995). For instance, shear tests on wheat kernels by Hourston et al., (Hourston et al., 2017) demonstrated that the force required for shearing varied significantly with tempering time (0 to 6h). Interestingly, changes in compression characteristics of intact wheat kernel with tempering time have been largely overlooked. This underscores the importance of studying the water uptake under differing tempering conditions and its impact on mechanical properties of wheat. Thus, the specific objectives of this study are (1) elucidate the influence of targeted tempering conditions on moisture diffusivity, specifically investigate how moisture diffusivity changes with varying tempering moisture content (2) characterize the variations in the mechanical properties of individual wheat kernels with tempering time; analyze how compressive force and elastic modulus evolve with tempering time.

## 5.2 Materials and Methods

### 5.2.1 Experimental design

A full factorial design with three independent variables (wheat class, tempering moisture, and tempering time) was employed for evaluating the viscoelastic properties of wheat kernels. The two classes of wheat, hard red spring (HRS) and hard red winter (HRW), selected for the study was obtained from Montana Flour and Grains (Fort Benton, Montana, USA). Moisture content (% wet basis) and tempering time were evaluated at three levels (14.0 %, 16.0%, 18.0%) and four durations (3, 6, 9, 12 h), respectively. Twenty kernels were analyzed under each experimental condition.

The moisture content of the samples was determined by oven method following ASABE Standard S352.2 (ANSI/ASABE, 2012) for whole kernels. The protein content of the samples was measured by AACC 46-30.01 (AACC, 2009).

### 5.2.2 Tempering

In the tempering process, water is added to the wheat to increase its moisture content to the predetermined level. The kernels are then stored for a specified time period to ensure the moisture uptake inside the kernels. In the study, the amount of water to be added to the kernels was calculated according to the following equation 5.1 (Kruszelnicka et al., 2022),

*Water added (ml)*

$$= \frac{\text{Mass of wheat} \times (\text{Final target moisture} - \text{Initial moisture content})}{(100 - \text{Final target moisture})}$$

Calculated amount of water was then added to 500 g of wheat kernels to raise their moisture content to the target values of 14.0%, 16.0% and 18.0%. After mixing thoroughly, the lot was divided into 100g batches and stored in sealed polyethylene bags for subsequent experiments.

The samples were maintained at a constant temperature of  $22.0 \pm 0.5$  °C throughout the

experiments. Equilibrium relative humidity, corresponding to the target moisture content of the tempered wheat was maintained in the storage chamber (Model I-36 VL, Pervical Scientific Inc., Iowa, USA). At every three-hour, a bag of conditioned wheat is chosen randomly from the lot for experimentation. Moisture content was measured at each sampling interval following standard protocol ASABE Standard S352.2 (ANSI/ASABE, 2012).

### 5.2.3 Geometric properties

Geometric properties of individual wheat kernels were measured using digital caliper (UltraTech, General Tools & Instruments, USA). Three principal axes of 20 randomly selected kernels (i.e., L: length, W: width and T: thickness) were measured before each uniaxial compression test. Equivalent diameter ( $D_p$ ) of the wheat kernels was calculated as per equation 5.2.

$$D_p = \left( \frac{L \times (W + T)^2}{4} \right)^{1/3}$$

### 5.2.4 Moisture migration

Moisture migration within wheat kernels occurs through diffusion (Li & Jiang, 2016). The analytical solution for the diffusion equation depends on the geometry and boundary conditions. The experiments to understand the moisture migration inside the kernels employed the following boundary and initial conditions:

- 1) Initial moisture is uniformly distributed throughout the kernel.
- 2) At  $t = 0$ , the surface moisture equilibrates with the surrounding environment, neglecting surface resistance.
- 3) For  $t > 0$ , the kernel surface maintains equilibrium with the surrounding environment, which is maintained at predetermined conditions.

- 4) The moisture content of the kernel approaches equilibrium at the end of the tempering process.

Other assumption in determining the effective moisture diffusivity of wheat are:

- 1) The kernels were maintained in an isothermal environment at  $22.0 \pm 0.5$  °C and heat transfer was neglected.
- 2) The tempering process has a negligible effect on the kernel's volume.
- 3) The composition of the kernel is uniform and is isotropic.

The general analytical solution of the diffusion equation (Eq. 5.3) can be represented in terms of moisture ratio as (Kang & Delwiche, 1999)

$$MR = \frac{m_t - m_{in}}{m_{eq} - m_{in}} = 1 - \sum_{n=1}^{\infty} \frac{6}{(n\pi)^2} \exp(-(n\pi)^2 F_o)$$

Where

MR = moisture ratio; a dimensionless quantity ranging between 0 and 1

$m_t$  = moisture content at time t (% , dry basis)

$m_{in}$  = initial moisture content of the wheat kernels (% , dry basis)

$m_{eq}$  = equilibrium moisture content of the kernel at its surface (% , dry basis)

$n = 1, 2, 3, \dots$

$F_o$  = Fourier number (Eq. 5.4)

$$F_o = \frac{D_{eff} t}{L_c^2}$$

Where

$D_{eff}$  = effective diffusivity ( $m^2/s$ )

t = time (s)

$L_c$  = characteristic length (m)

For a sphere,  $L_c$  = radius of the sphere.

The analytical solution for the moisture migration inside the single kernel considering spherical diffusion equation (Eq. 5.5) with zero surface resistance

$$MR = 1 - \sum_{n=1}^{\infty} \frac{6}{(n\pi)^2} \exp\left(- (n\pi)^2 \frac{D_{eff} t}{r^2}\right)$$

It is evident that the first term of the series will dominate the rest. Thus, the natural logarithmic form will be as follows (Eq. 5.6)

$$\ln(MR) = \ln(0.608) - \frac{9.8696 D_{eff} t}{r^2}$$

The effective diffusivity was calculated from the slope of  $\ln(MR)$  versus time plot (Eq. 5.7 – 5.8).

$$\ln(MR) = -0.4975 - \frac{9.8696 D_{eff} t}{r^2}$$

$$D_{eff} = \frac{b}{(9.8696/r^2)}$$

Where the radius  $r$  is determined based on the equivalent diameter ( $D_p$ ) of the wheat kernel and  $b$  is the slope of  $\ln(MR)$  versus time plot.

### 5.2.5 Viscoelastic characterization of the wheat kernels

A quasi static compression test was performed on wheat kernels to evaluate their viscoelastic properties using a texture analyzer (TA-XT2, Stable Microsystems, UK). The compressive load was applied to the samples using a cylindrical probe, TA-25 (diameter = 50.8 mm and height = 20 mm). Prior to testing, the conditioned kernels were placed in their most stable position, with the crease side facing down. The crosshead velocity for pre-test, test, and post-test velocities were maintained at 0.1mm/s. This velocity and placement condition ensured that the wheat

kernels did not produce any lateral movement during the compression and remained stationary (Han et al., 2021).

The technique described by Figueroa and co-authors (Ponce-García et al., 2008) was employed for determining the contact area of individual kernels. Briefly, the load bearing surface of the kernel was inked and placed on to the plate. A piece of paper was taped on to the loading face of the probe. During loading, the ink impression of the loading area was transferred onto the paper. This impression was digitized, and the contact area was calculated using Image J software (Schneider et al., 2012).

Compression tests were performed, generating force- deformation curve of the kernels. The force - deformation data obtained from uniaxial compression of the samples using texture analyzer was utilized to evaluate the viscoelastic properties. Modulus of elasticity (Young's modulus) was determined from the stress- strain curve within the initial linear region (5% deformation) using the equation (Eq 5.9):

$$E = \frac{\sigma}{\varepsilon}$$

where  $\sigma$  (force/area) is normal stress and  $\varepsilon$  is the strain. Here (Eq. 5.10),

$$\varepsilon = \left[ \frac{(T_0 - T_f)}{T_0} \right] \times 100$$

where  $T_0$  and  $T_f$  are the initial and final thickness of the kernel.

The viscoelastic behavior of wheat kernels was evaluated from the force - deformation curve obtained from the compression study. Total work ( $W_t$ , N.mm) was determined by calculating the area enclosed within the loading curve. The area under the unloading curve represented the elastic work ( $W_e$ , N.mm), and the difference between the total work and the elastic work was termed the plastic work ( $W_p$ , N.mm) according to the equation 5.11:

$$W_p = W_t - W_e$$

A schematic representation of the compression study is illustrated in Fig 5.1.

### 5.2.6 Statistical analysis

All statistical analyses were carried out using OriginPro 2023b (OriginLab Corporation, USA). ANOVA was conducted at 95% confidence interval, and Tukey's honest significance test ( $p < 0.05$ ) was used to evaluate the differences between the treatment means. Additionally, principal component analysis (PCA) and k – means clustering were performed on the data.

## 5.3 Results

The physicochemical characteristics of the selected wheat kernels are detailed in Table 5.1. No significant differences were observed in kernel dimensions among the wheat classes. Initial moisture content was 8.6 % and 7.8% (wet basis) for HRW and HRS, respectively. The protein content exhibited significant variation, with HRW at 10.15% and HRS at 16.25%, making it the primary reason for choosing these samples for the study. Mechanical properties also displayed marked differences. HRS samples demonstrated higher compression force (116.8 N) compared to HRW samples (72.8 N). Elastic modulus of the samples was in the range reported in literature (Escalante-Aburto et al., 2023; Figueroa et al., 2011; Ponce-García et al., 2008).

### 5.3.1 Changes in physical and mechanical properties with tempering

Tempering conditions significantly influenced the physical properties of the kernels (Table 5.2). HRW kernels exhibited larger dimensions compared to HRS kernels, particularly in compression area. For instance, the compression area for HRS and HRW samples were 2.49 and 2.65 mm<sup>2</sup>, respectively (Table 5.2) on tempering the kernels to 16% for 12 h. The compression area of both HRW and HRS kernels increased with moisture content ( $p < 0.05$ ). With higher moisture content (18%), the kernel undergoes greater deformation under the specified force, resulting in an

increased deformation area. When the HRW kernels were tempered to 18%, the compression area increased to 3.14 mm<sup>2</sup> as opposed to the control (un-tempered) samples, which had a compression area of 2.98 mm<sup>2</sup> (Table 5.1 and Table 5.2). These changes can be correlated to the alterations observed in the effective diffusivities of the kernels. The diffusivities are influenced by moisture content (Gulati & Datta, 2013; Maroulis et al., 2001) and wheat type (Li & Jiang, 2016).

Furthermore, the diffusivity of the kernels increased when moisture content was increased from 14% to 16% (Table 5.5). This implies that moisture movement within the kernels accelerate at higher moisture contents. For instance, the effective moisture diffusivity of HRW was  $1.63 \times 10^{-11}$  m<sup>2</sup>/s at 14% increasing to  $2.45 \times 10^{-11}$  m<sup>2</sup>/s at 16%. However, the diffusivity rose to  $2.81 \times 10^{-11}$  m<sup>2</sup>/s as the tempering moisture content was further increased to 18%. Despite the increase, the change in effective diffusivities was not statistically significant ( $p > 0.05$ ). Effective moisture diffusivities depend on moisture concentration. At higher tempering moisture levels, the elevated initial moisture on the surface enhances moisture movement towards the kernel's interior, consequently increasing the effective diffusivity.

Moisture content and tempering time significantly influenced the peak compression force and maximum compressive stress of the kernels (Table 5.2). In general, the force required to break the kernels decreased with increasing moisture content and time for all studied samples. Higher moisture content plasticized the kernels, leading to disintegration at a lower force. For instance, the compression force for HRW kernels decreased from 51.65 to 40.23 N as the moisture content increased from 14% to 18%. This observation is consistent with findings of other authors (Bargale et al., 1995; Bechtel et al., 2009; Haddad et al., 2001) who have noted that wheat kernels transition from elastic – plastic state at 14% moisture to a plastic viscous state at

moisture levels above 15%. Moreover, this can be associated with tempering the hard wheat kernels to achieve moisture levels in the range of 16 – 16.5 % before milling.

Furthermore, over time the moisture migration within the kernel altered the mechanical properties of the bran, its associated layers, and the endosperm facilitating easier kernel breakage with extended tempering time. For example, increasing the tempering time of HRS kernels from 3 to 12 h resulted in a decrease in compression force from 58.65 N to 52.01 N for kernels tempered at 14% moisture content. A similar trend was observed for other studied moisture levels where the compression force for HRW kernels tempered to 16% decreased from 48.71 N to 45.28 N.

The elastic modulus of the HRS and HRW varied in the range of 114.96 – 192.17 MPa and 89.15 – 155.79 MPa, respectively. A noticeable decline in modulus of elasticity was observed as the moisture content was increased from 14% to 18%. This reduction in elasticity with rising moisture content aligns with the findings reported in literature (Escalante-Aburto et al., 2023; Figueroa et al., 2011; Ponce-García et al., 2008, 2013). It is important to note that the elasticity values obtained in our studies are comparatively lower than those documented in literature. For instance, in the studies conducted by Figueroa et al., (Figueroa et al., 2011) the modulus of elasticity of HRW wheat (cultivar: Rayon) decreased from 116.1 MPa to 52.4 MPa when its moisture content increased from 13 % to 19%. Similarly, according to Ponce-García and co-authors (Ponce-García et al., 2013), the values decreased from 394.8 MPa to 99.2 MPa with an increase in moisture levels from 9.3 to 22.5%. The variations in wheat type, moisture content, loading rate and experimental methodologies present challenges in directly comparing our results with the existing literature.

Additionally, the experiments revealed a significant decrease in elasticity of the kernels with extended tempering time across all moisture levels. For example, at 14% moisture content, the elasticity of HRS kernels decreased by 14% with the increase in tempering time from 3h to 12h. This implies that, as the tempering time extends to 12h, the kernels become less elastic, requiring 14% less force to fracture compared to the force needed at 3h. Moreover, the changes in elasticity over tempering time were more pronounced at 14% moisture content compared to 18%.

### **5.3.2 Viscoelastic properties of wheat kernels**

Figure 5. 2 illustrates the changes in elastic and plastic work for HRS and HRW samples tempered to different moisture contents for 12h. The area encompassed by the plastic region, representing plastic work, increased with moisture content for both kernel types. Tempering wheat kernels to higher moisture levels reduced the peak force and elastic work.

Elastic materials undergo immediate deformation when stress is applied, and the strain disappears upon stress removal, resulting in complete recovery to the original state. In contrast, plastic materials do not revert to their initial state after stress removal, leading to permanent deformation of the wheat kernel (Foster et al., 2006). Both HRW and HRS kernels exhibited notably high elastic work at 14% moisture content, which gradually decreased with increasing moisture content (Table 5.3). This suggests that, at the studied deformation levels, the changes in the kernels are predominantly elastic and recoverable at lower moisture levels. Specifically, the elastic work of HRS samples decreased from 11.08 Nmm to 6.38 Nmm as the moisture content increased from 14 to 18%. A similar trend was observed for the HRW samples, with the elastic work decreasing from 8.75 Nmm to 5.42 Nmm (Escalante-Aburto et al., 2023; Figueroa et al., 2011). Interestingly, elastic work also exhibits a decreasing trend with tempering time. At 16% moisture content, for instance, the elastic work of HRS kernels decreased from 10.18 Nmm to 9

Nmm over the tempering time (3h – 12h). In other words, the elastic recovery from the kernels significantly decreases as the tempering time increases from 3h to 12h. This highlights the significant role of time in enhancing kernel friability.

During the initial tempering hours, plastic work was negligible, especially for kernels tempered to 14% moisture content, indicating the difficulty in breaking the kernels at this stage. This was particularly evident in HRS kernels, where no plastic work was observed at 14% moisture content (fig. 5.2a). However, a substantial increase in plastic work (0.83 Nmm to 1.58 Nmm) occurred when the kernels were tempered to 18%. At higher moisture content, plastic work increased significantly, accompanied by a notable decrease in elastic work. These observations suggest that at lower moisture levels, kernel breakage can be achieved by extending the tempering time, allowing for adequate moisture migration, and facilitating easier deformation of the kernels. Additionally, the inherent differences in the kernel texture of HRW and HRS contribute to variations in their viscoelastic properties (Bechtel et al., 2009; Ponce-García et al., 2013).

Table 5.4 represents the results of ANOVA, indicating statistical significance for the three independent variables: wheat class, moisture and tempering time in the viscoelastic properties. Moisture content was the most influential factor affecting peak compression force and plastic work. On the other hand, wheat class influenced the elastic modulus and elastic work. In comparison, tempering time had a relatively lesser effect on the studied viscoelastic properties. Fig. 5.3 illustrates the distribution of the studied viscoelastic properties on the plane defined by PC1 and PC2. These two variables, PC1 and PC2, collectively account for 86.55% of the variability in the observations. The ellipses in the figure indicate significance at a 95% confidence interval for each wheat class. While differences in the viscoelastic characteristics of

HRW and HRS are evident (Fig. 5.3), there is an overlap of the ellipses, suggesting that distinguishing between the classes can be challenging under the studied conditions.

### 5.3.3 Changes in compressibility with tempering

Peak force required to break the wheat kernels was found to decrease with tempering time. This change in force was found to follow first order kinetics with tempering time (Eq. 5.12).

$$F_t = F_0 e^{-kt}$$

Where  $F_t$  and  $F_0$  are the force required to break the kernels after tempering for  $t$  and 0 hours (un-tempered conditions), respectively,  $k$  is the rate constant ( $\text{h}^{-1}$ ) and  $t$  is the tempering time in h.

Rate constant for compressibility was calculated from the logarithmic plot of relative force ( $F_t/F_0$ ) against time. It was found that the regression coefficient for the  $k$  calculation was greater than 0.87. Table 5.5 shows the rate constant,  $k$  ( $\times 10^{-3} \text{ h}^{-1}$ ) obtained for all tempering conditions. The rate constant for compressibility is noted to decrease with an increase in tempering moisture. Specifically, at higher tempering moisture content, the force required to break the kernels exhibits a relatively slow variation over time. For instance, the rate constant for HRS decreased from  $0.0057 \text{ h}^{-1}$  to  $0.002 \text{ h}^{-1}$  as the moisture content varied from 14% to 18%.

Additionally, the rate constant was higher for HRW in comparison to HRS. In other words, at any given moisture content, HRW samples exhibit higher rate of change in compressibility. For example, at 14% the  $k$  value was  $0.0057 \text{ h}^{-1}$  for HRS whereas it was  $0.0066 \text{ h}^{-1}$  for HRW. This is analogous to the diffusivities of the kernels at different moisture content.

## 5.4 Discussion

Wheat kernels are predominantly composed of starchy endosperm, enveloped by various outer layers, including the aleurone layer, testa, and pericarp (Tu & Li, 2020). The biomechanical properties of these outer layers are distinct, influenced by factors such as cell structure,

composition, thickness, and adhesion. In the process of wheat milling, these layers are removed to obtain flour, and the efficiency of endosperm recovery relies on the mechanical property differences between the endosperm and bran layers. Tempering, involving the addition of water to the kernels, enhances these mechanical differences, thereby facilitating endosperm separation. The migration of moisture through the bran layers is a critical factor in achieving effective bran-endosperm separation. Elevated moisture on the outer layers accelerate moisture transfer (Table 5.5), leading to alterations in concentration gradients and modifications to the mechanical properties of the layers. Increasing moisture content induces changes in intercellular distance, resulting in grain volume expansion and improved starch mobility. This, in turn, enhances plasticity and reduces hardness (Qiao et al., 2022). At higher moisture levels, kernels undergo plasticization, resulting in a diminished rate of change in compressive force, as evidenced by the rate constant (table 5). The plasticization effect of moisture is attributed to the weakening of dipole-dipole interactions and hydrogen bonds, both intramolecular and intermolecular. Water molecules disrupt the attractive forces between biopolymers such as polysaccharides and proteins, facilitating increased molecular motion and, consequently, reducing compression force and elastic modulus. This observation is supported by the documented reduction in the elastic modulus of bran layers with increasing moisture content (Hemery et al., 2010). Moreover, moisture content significantly influences the fracture pattern of bran layers, with outer layers fracturing before the inner layer at moisture levels below 16%. Additionally, reduced hardness not only alters the compression force and but also reduces the energy required for milling (Dziki et al., 2014).

According to Qiao et al. (Qiao et al., 2022), hardness and elasticity of kernel are determined by protein content, whereas viscosity and deformation are linked to starch molecules. During

tempering, as kernels absorb moisture, the pore structure around the starch undergoes modification, impacting its viscosity and deformation. Moreover, the breakage resistance of grains is influenced by factors such as porosity, the number of closed pores, and the surface area of closed pores (Dong et al., 2020). These factors exhibit variations with moisture migration within the kernels, thereby affecting the mechanical properties as tempering progresses. Over time, moisture gradually permeates the inner bran layers, leading to alterations in their mechanical characteristics. This is evident in the observed decrease in compression force and stress characteristics of kernels with increasing tempering time.

HRS and HRW wheat kernels display distinct physicochemical and mechanical characteristics. HRS wheat kernels, characterized by the Pina-D1b (a-null) hardness allele, exhibit greater hardness compared to HRW kernels with the Pinb-D1b allele (Morris & Massa, 2003). These genetic variations not only alter hardness but also impact compressive force and the area under the force-deformation curve. Moreover, textural variations arise from starch-protein interactions, environmental factors like drought and rainfall during growth, and nitrogen availability during kernel development. These differences are reflected in the moisture diffusivities and mechanical properties of the examined wheat kernels. The diffusivity of kernels varies with kernel hardness and vitreousness in wheat endosperm (Glenn & Johnston, 1994; Mayolle et al., 2012). Glenn et al. (Glenn et al., 1991) reported that hard wheats are more responsive to moisture content variations. In our study, HRW kernels exhibited higher sensitivity in mechanical properties to moisture content compared to HRS kernels, as indicated by the rate constant. The lower protein content of HRW wheat results in reduced grain hardness or vitreousness, correlating with higher water uptake (Molina-Cano et al., 2002). However, it's important to note that the reported

changes in diffusivities are not statistically significant within the wheat class due to the narrow range of moisture levels studied.

## **5.5 Conclusions**

The present study investigated the influence of tempering time and moisture content on the mechanical properties and diffusivity of HRW and HRS wheat kernels. The findings revealed that tempering time significantly impact the compressive strength of the kernels. While the conclusion is based on a relatively small sample size, the observed trends suggests that the conclusions can be extended to other wheat classes. Additionally, the study demonstrated that HRW and HRS samples exhibit similar yet distinct changes in the compressibility characteristics and viscoelastic properties. A novel finding of the work is that kernel compressibility follows first order kinetics. Furthermore, changes in kernel diffusivity were observed with respect to tempering moisture content. These findings provide valuable insights for optimizing the tempering process by reducing tempering time, ultimately reducing total energy requirements and improving overall efficiency.

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## Tables

**Table 5.1. Physical and mechanical properties of un-tempered wheat (control) samples**

| Properties                                    |                   | Hard Red Winter (HRW) | Hard Red Spring (HRS) |
|-----------------------------------------------|-------------------|-----------------------|-----------------------|
| Kernel dimensions:                            | Length (L), mm    | 6.16 (0.3)            | 5.62 (0.2)            |
|                                               | Width (W), mm     | 2.91 (0.1)            | 2.99 (0.1)            |
|                                               | Thickness (T), mm | 2.67 (0.1)            | 2.76 (0.2)            |
| Equivalent diameter ( $D_p$ ), mm             |                   | 3.63 (0.08)           | 3.59 (0.09)           |
| Moisture content (% , wet basis)              |                   | 8.58 (0.11)           | 7.79 (0.12)           |
| Protein content (% , 14% moisture basis)      |                   | 10.19 (0.05)          | 16.25 (0.07)          |
| Compression area, mm <sup>2</sup>             |                   | 2.98 (0.7)            | 2.05 (0.3)            |
| Compression force, N                          |                   | 72.78 (8.7)           | 116.8 (11.8)          |
| Final stress ( $\sigma$ ), N/ mm <sup>2</sup> |                   | 24.42 (5.3)           | 56.97 (12.0)          |
| Elastic modulus (E), MPa                      |                   | 191.08 (35.3)         | 323.21 (35.8)         |

Measurements are reported as mean (standard deviation), representing the average of 20 readings.

**Table 5.2. Effect of tempering conditions on the physical and mechanical properties of wheat**

| Wheat | Moisture<br>(%, wet<br>basis) | Time,<br>h | Compression<br>area, mm <sup>2</sup> | Compression<br>force, N    | Final stress,<br>N/mm <sup>2</sup> | Elastic modulus,<br>MPa      |
|-------|-------------------------------|------------|--------------------------------------|----------------------------|------------------------------------|------------------------------|
| HRW   | 14                            | 3          | 2.25 (0.6) <sup>D</sup>              | 51.65 (6.5) <sup>A</sup>   | 22.76 (6.9) <sup>A</sup>           | 155.79 (47.5) <sup>A</sup>   |
|       |                               | 6          | 2.3 (0.5) <sup>D</sup>               | 49.68 (9.4) <sup>A</sup>   | 21.32 (4.2) <sup>AB</sup>          | 149.39 (31.3) <sup>AB</sup>  |
|       |                               | 9          | 2.48 (0.4) <sup>CD</sup>             | 49.55 (8.0) <sup>A</sup>   | 20.45 (5.5) <sup>AB</sup>          | 135.26 (36.1) <sup>AB</sup>  |
|       |                               | 12         | 2.52 (0.5) <sup>BCD</sup>            | 44.38 (9.4) <sup>ABC</sup> | 20.80 (6.1) <sup>AB</sup>          | 134.96 (38.3) <sup>AB</sup>  |
|       | 16                            | 3          | 2.57 (0.4) <sup>BCD</sup>            | 48.71 (9.4) <sup>A</sup>   | 19.16 (4.6) <sup>ABC</sup>         | 125.57 (30.2) <sup>ABC</sup> |
|       |                               | 6          | 2.57 (0.5) <sup>BCD</sup>            | 48.00 (8.9) <sup>AB</sup>  | 18.76 (4.3) <sup>ABC</sup>         | 123.26 (29.0) <sup>ABC</sup> |
|       |                               | 9          | 2.62 (0.4) <sup>ABCD</sup>           | 46.43 (7.1) <sup>ABC</sup> | 18.62 (4.5) <sup>ABC</sup>         | 121.51 (30.0) <sup>BCD</sup> |
|       |                               | 12         | 2.65 (0.4) <sup>ABCD</sup>           | 45.28 (5.4) <sup>ABC</sup> | 17.77 (4.0) <sup>BCD</sup>         | 118.42 (26.6) <sup>BCD</sup> |
|       | 18                            | 3          | 2.74 (0.6) <sup>ABCD</sup>           | 40.23 (6.0) <sup>BC</sup>  | 15.08 (3.9) <sup>CDE</sup>         | 99.71 (25.8) <sup>CDE</sup>  |
|       |                               | 6          | 3.05 (0.7) <sup>AB</sup>             | 39.91 (7.0) <sup>BC</sup>  | 13.61 (3.0) <sup>DE</sup>          | 89.40 (19.3) <sup>DE</sup>   |
|       |                               | 9          | 3.01 (0.6) <sup>ABC</sup>            | 38.39 (6.5) <sup>C</sup>   | 13.26 (3.3) <sup>DE</sup>          | 89.19 (25.4) <sup>DE</sup>   |
|       |                               | 12         | 3.14 (0.6) <sup>A</sup>              | 38.38 (7.80) <sup>C</sup>  | 12.56 (3.5) <sup>E</sup>           | 89.15 (21.0) <sup>E</sup>    |
| HRS   | 14                            | 3          | 1.91 (0.27) <sup>b</sup>             | 58.65 (11.8) <sup>a</sup>  | 28.75 (4.7) <sup>a</sup>           | 192.17 (32.1) <sup>a</sup>   |
|       |                               | 6          | 2.11 (0.27) <sup>ab</sup>            | 56.05 (6.6) <sup>a</sup>   | 28.01 (5.7) <sup>a</sup>           | 185.45 (38.6) <sup>a</sup>   |
|       |                               | 9          | 2.13 (0.43) <sup>ab</sup>            | 54.2 (6.4) <sup>a</sup>    | 26.94 (4.8) <sup>ab</sup>          | 179.65 (33.1) <sup>a</sup>   |
|       |                               | 12         | 2.15 (0.46) <sup>ab</sup>            | 52.01 (8.6) <sup>ab</sup>  | 24.99 (5.7) <sup>ab</sup>          | 164.86 (38.6) <sup>ab</sup>  |
|       | 16                            | 3          | 2.18 (0.23) <sup>ab</sup>            | 56.25 (8.8) <sup>a</sup>   | 25.73 (3.3) <sup>ab</sup>          | 175.86 (23.6) <sup>ab</sup>  |
|       |                               | 6          | 2.31 (0.45) <sup>ab</sup>            | 55.66 (5.6) <sup>a</sup>   | 25.05 (5.6) <sup>ab</sup>          | 168.94 (39.9) <sup>ab</sup>  |
|       |                               | 9          | 2.4 (0.56) <sup>a</sup>              | 54.57 (8.7) <sup>a</sup>   | 23.87 (6.2) <sup>abc</sup>         | 159.51 (41.3) <sup>ab</sup>  |

|    |    |                          |                           |                            |                              |
|----|----|--------------------------|---------------------------|----------------------------|------------------------------|
|    | 12 | 2.49 (0.41) <sup>a</sup> | 52.15 (7.5) <sup>ab</sup> | 21.50 (4.4) <sup>bcd</sup> | 143.01 (27.9) <sup>bcd</sup> |
| 18 | 3  | 2.49 (0.68) <sup>a</sup> | 44.44 (9.5) <sup>bc</sup> | 19.27 (6.5) <sup>cd</sup>  | 127.53 (43.6) <sup>cd</sup>  |
|    | 6  | 2.50 (0.35) <sup>a</sup> | 43.98 (7.7) <sup>bc</sup> | 17.97 (3.9) <sup>d</sup>   | 118.75 (25.7) <sup>d</sup>   |
|    | 9  | 2.51 (0.51) <sup>a</sup> | 42.94 (7.7) <sup>c</sup>  | 17.46 (3.6) <sup>d</sup>   | 116.99 (26.8) <sup>d</sup>   |
|    | 12 | 2.55 (0.56) <sup>a</sup> | 42.79 (5.8) <sup>c</sup>  | 17.46 (3.8) <sup>d</sup>   | 114.96 (23.2) <sup>d</sup>   |

Measurements are reported as mean (standard deviation), representing the average of 20 readings. Values with the same case letters within a wheat class are not statistically different ( $\alpha = 0.05$ ).

**Table 5.3. Effect of tempering conditions on the viscoelastic properties of wheat**

| Wheat | Moisture<br>(%, wet basis) | Time (h) | Elastic work (N.mm)       | Plastic work (N.mm)        |
|-------|----------------------------|----------|---------------------------|----------------------------|
| HRW   | 14                         | 3        | 8.75 (1.8) <sup>A</sup>   | -                          |
|       |                            | 6        | 8.27 (2.5) <sup>A</sup>   | -                          |
|       |                            | 9        | 8.08 (1.9) <sup>A</sup>   | 0.22 (1.4) <sup>CD</sup>   |
|       |                            | 12       | 6.80 (2.3) <sup>ABC</sup> | 0.45 (0.3) <sup>BCD</sup>  |
|       | 16                         | 3        | 8.00 (2.4) <sup>A</sup>   | 0.18 (0.9) <sup>CD</sup>   |
|       |                            | 6        | 7.82 (2.4) <sup>AB</sup>  | 0.30 (2.7) <sup>CD</sup>   |
|       |                            | 9        | 7.29 (1.8) <sup>ABC</sup> | 0.57 (0.9) <sup>ABCD</sup> |
|       |                            | 12       | 6.90 (1.5) <sup>ABC</sup> | 0.58 (1.1) <sup>ABCD</sup> |
|       | 18                         | 3        | 5.82 (1.4) <sup>BC</sup>  | 1.47 (0.8) <sup>ABC</sup>  |
|       |                            | 6        | 5.75 (1.6) <sup>C</sup>   | 1.70 (0.7) <sup>AB</sup>   |
|       |                            | 9        | 5.46 (1.7) <sup>C</sup>   | 1.73 (0.7) <sup>AB</sup>   |
|       |                            | 12       | 5.42 (1.4) <sup>C</sup>   | 1.86 (0.7) <sup>A</sup>    |
| HRS   | 14                         | 3        | 11.08 (3.6) <sup>a</sup>  | -                          |
|       |                            | 6        | 10.09 (1.9) <sup>a</sup>  | -                          |
|       |                            | 9        | 9.59 (1.7) <sup>a</sup>   | -                          |
|       |                            | 12       | 8.88 (2.4) <sup>ab</sup>  | -                          |
|       | 16                         | 3        | 10.18 (2.6) <sup>a</sup>  | 0.13 (0.9) <sup>cde</sup>  |
|       |                            | 6        | 10.08 (1.7) <sup>a</sup>  | 0.37 (0.9) <sup>bcd</sup>  |
|       |                            | 9        | 9.67 (2.5) <sup>a</sup>   | 0.43 (0.7) <sup>bcd</sup>  |
|       |                            | 12       | 9.00 (2.2) <sup>ab</sup>  | 0.46 (0.7) <sup>bcd</sup>  |

|    |    |                          |                           |
|----|----|--------------------------|---------------------------|
| 18 | 3  | 7.00 (2.3) <sup>bc</sup> | 0.83 (0.9) <sup>abc</sup> |
|    | 6  | 6.81 (2.0) <sup>bc</sup> | 0.91 (1.5) <sup>abc</sup> |
|    | 9  | 6.64 (1.9) <sup>bc</sup> | 1.21 (0.7) <sup>ab</sup>  |
|    | 12 | 6.38 (1.5) <sup>c</sup>  | 1.58 (0.8) <sup>a</sup>   |

Measurements are reported as mean (standard deviation), representing the average of 20 readings. Values with the same case letters within a wheat class are not statistically different ( $\alpha = 0.05$ ).

**Table 5.4. ANOVA for evaluated mechanical properties of wheat kernels as a function of wheat class, moisture and tempering time and their interactions**

| Component       | df | Compressive force |                | Elastic modulus |                | Elastic work   |                | Plastic work   |                |
|-----------------|----|-------------------|----------------|-----------------|----------------|----------------|----------------|----------------|----------------|
|                 |    | <i>F value</i>    | <i>P value</i> | <i>F value</i>  | <i>P value</i> | <i>F value</i> | <i>P value</i> | <i>F value</i> | <i>P value</i> |
| Wheat class (C) | 1  | 68.15             | <0.0001        | 136.83          | <0.0001        | 80.24          | <0.0001        | 11.85          | 0.0006         |
| Moisture (M)    | 2  | 82.64             | <0.0001        | 122.91          | <0.0001        | 79.53          | <0.0001        | 80.58          | <0.0001        |
| Time (T)        | 3  | 5.35              | 0.0013         | 5.95            | 0.0006         | 6.48           | 0.0003         | 3.04           | 0.029          |
| C × M           | 2  | 1.65              | 0.194          | 1.06            | 0.346          | 2.99           | 0.051          | 2.21           | 0.111          |
| C × T           | 3  | 0.18              | 0.911          | 0.57            | 0.636          | 0.38           | 0.769          | 1.00           | 0.392          |
| M × T           | 6  | 0.63              | 0.705          | 0.38            | 0.892          | 0.75           | 0.606          | 0.41           | 0.872          |
| C × M × T       | 6  | 0.39              | 0.888          | 1.24            | 0.285          | 0.55           | 0.773          | 0.40           | 0.878          |

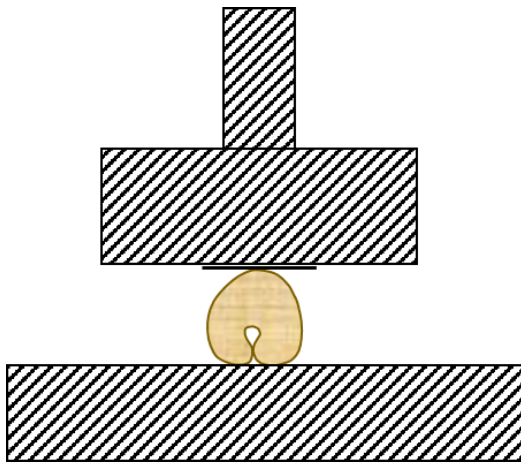
**Table 5.5. Effective diffusivity and rate constants with tempering**

| <b>Moisture</b><br><br>(%, wet basis) | <b>Effective diffusivity (<math>D_{\text{eff}}</math>, <math>10^{-11} \text{ m}^2 \text{ s}^{-1}</math>)</b> |                          | <b>Rate constant (<math>k</math>, <math>10^{-3} \text{ h}^{-1}</math>)</b> |                            |
|---------------------------------------|--------------------------------------------------------------------------------------------------------------|--------------------------|----------------------------------------------------------------------------|----------------------------|
|                                       | <b>HRS</b>                                                                                                   | <b>HRW</b>               | <b>HRS</b>                                                                 | <b>HRW</b>                 |
| 14                                    | 2.84 (0.05) <sup>a</sup>                                                                                     | 1.63 (0.08) <sup>A</sup> | 5.7 (0.00022) <sup>a</sup>                                                 | 6.6 (0.00022) <sup>A</sup> |
| 16                                    | 2.92 (0.04) <sup>a</sup>                                                                                     | 2.45 (0.09) <sup>A</sup> | 3.6 (0.00081) <sup>b</sup>                                                 | 3.7 (0.00036) <sup>B</sup> |
| 18                                    | 3.54 (0.06) <sup>a</sup>                                                                                     | 3.81 (0.04) <sup>A</sup> | 2.0 (0.00038) <sup>c</sup>                                                 | 2.6 (0.00072) <sup>C</sup> |

Measurements are reported as mean (standard deviation), representing the average of 3 readings. Values with the same case letters within a wheat class are not statistically different ( $\alpha = 0.05$ ).

## Figures

**a**



**b**

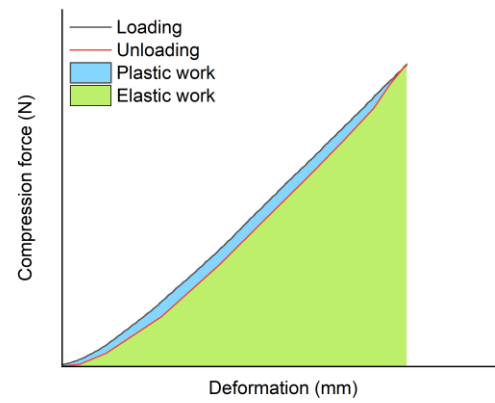


**Figure 5.1. Schematic showing the (a) uniaxial compression of wheat kernel (b) load deformation curve of compression**

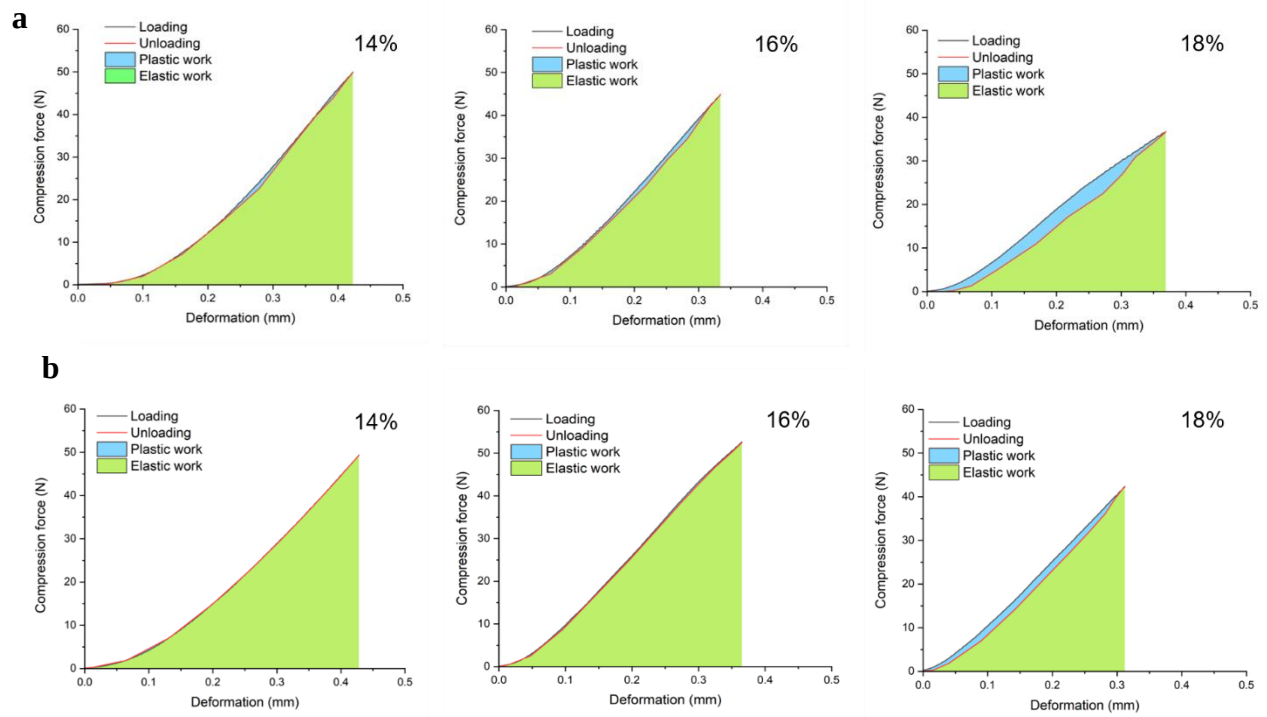


**Figure 5.2. Typical force – deformation curve of (a) hard red spring, HRS and (b) hard red winter HRW tempered to moistures 14.0 %, 16.0 % and 18.0 % for 12h.**

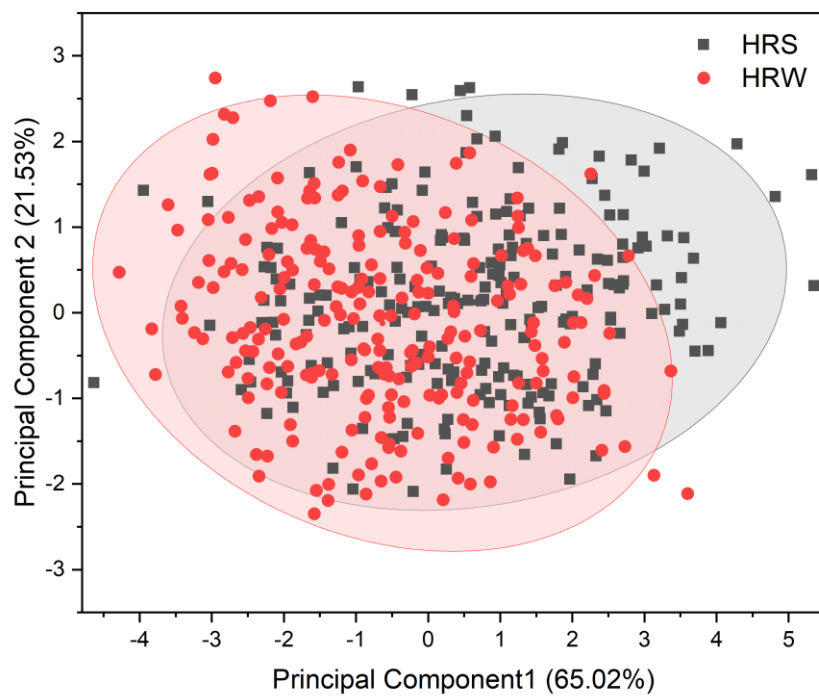


**Figure 5.3. Principal component analysis (PCA) score plot for viscoelastic properties of hard red spring (HRS) and hard red winter (HRW) wheat**

## **Chapter 6 Investigating the contribution of blending on the dough rheology of roller milled hard red wheat<sup>3</sup>**

### **Abstract**

The flour functionality and particle size distribution of wheat flour obtained on roller milling are dependent on the type of wheat, tempering conditions, and milling conditions. In this study, the impact of the tempering conditions (moisture and time) on the chemical and rheological properties of flour from blends of hard red wheats were analyzed. The wheat blends B1-25:75 [hard red spring (HRS): hard red winter (HRW)], B2-50:50, and B3-75:25, tempered to 14%, 16%, and 18% for 16, 20, and 24 h, were milled using a laboratory-scale roller mill (Buhler MLU-202). Protein, damaged starch, and particle characteristics were influenced by blending, tempering, and milling streams. For all the blends, the protein content varied significantly among the break flour streams; the damaged starch content varied greatly in the reduction streams. The increased damaged starch content of the reduction streams proportionally increased water absorption (WA). Higher proportions of HRS in the blends significantly decreased the pasting temperature of the dough, as measured using Mixolab. Principal component analysis proved that the protein content was the key determinant in particle characteristics, WA, and pasting properties of the flour, especially in blends with a higher proportion of HRS.

### **6.1 Introduction**

Nearly 20% of humans' calorific intakes worldwide are dependent on wheat (Hermans et al., 2021). Grain is consumed globally in different forms, such as leavened and unleavened bread,

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cakes, cookies, and pasta. Wheat flour is the main ingredient in these products. Therefore, it is necessary to recover flour of desirable processing quality. The process involved in the extraction of flour from kernels is termed wheat milling. During milling, the starchy endosperms of wheat kernels are separated from their outer layers (bran) and are reduced to flour. Factors contributing to efficient separation depend on the kernel quality and processing conditions. Flour quality is determined to a great extent by the type of wheat; however, the processing conditions (mill settings and tempering conditions) can also influence the physicochemical properties and particle characteristics of the flour (Baasandorj et al., 2015; Brüttsch et al., 2017; Campbell, 2007). For instance, the setup and environmental conditions of the mill can determine up to 25% of the functionality of flour; the remaining 75% is dependent on wheat quality (Posner, 2009).

According to (Campbell, 2007), the two key tools for ensuring consistent flour quality are wheat tempering and blending. Tempering is the process of conditioning wheat kernels for milling through the controlled addition of water followed by a resting period. The process is essential to exaggerate the friability differences between endosperm, germ, and bran (Posner, 2009). This mellows the endosperm and toughens the bran of wheat kernel to increase the efficiency of milling (Abo-Dief et al., 2019). The factors influencing the rate of moisture uptake by wheat kernels are the kernel properties, temperature, tempering time, and initial moisture content of wheat (Abo-Dief et al., 2019; Kweon et al., 2009). The flour extraction rate, composition, and functionality are altered by the tempering conditions. For instance, the flour yield, ash content, and functionality of soft wheat flour can be modified by increasing the tempering time from 3 to 24 h (Kweon et al., 2009). Similarly, tempering moisture alters the granulometric composition of flour (Fang & Campbell, 2003) and the rate of flour extraction (Hook et al., 1982), and influences energy consumption during the milling process (Warechowska et al., 2016).

In general, the quality of wheat is determined to a great extent by the environment and management practices (Raj et al., 2023; Rozbicki et al., 2015; Tian et al., 2022; Vazquez et al., 2019). These factors result in wheat (of any variety) exhibiting a range of quality characteristics. Variations in quality even within same variety compel millers to resort to blending to ensure consistent quality. Blending is defined as the process of mixing two or more wheat varieties or classes in a given ratio to obtain a wheat mixture which yields desired flour functionality after milling (Alfin, 2019). The process is necessary to ensure consistency in flour quality and cost optimization (Alfin, 2019; Li et al., 2014a). In practice, wheat of different qualities is mixed during blending to obtain flour of desirable quality (Hayta & Çakmakli, 2001). The wheat varieties chosen for blending might vary in physical properties, not simply in chemical composition. This can affect the granulometric composition of the flour, and therefore the quality. Mostly, the published literature focuses on optimizing blending in terms of the final flour quality and cost of operation (Hayta & Çakmakli, 2001; Li et al., 2014a; Noor et al., 2022). Additionally, wide variability exists in the composition and rheological properties of flour obtained from different milling streams (Pojić et al., 2014; Prabhasankar et al., 2000; Rani et al., 2001). This also increases the possibility of modifying the final product quality by blending flour from different streams. Hence, the final flour quality can be altered by blending, modifying the tempering conditions, and adjusting mill operational parameters such as the roll, roll speed, and roll differential. Thus, the blending process plays a significant role in the wheat supply chain, and is vital in ensuring profitability of the milling process (Li et al., 2014b).

Although there have been numerous studies on the impact of tempering on flour quality and biochemical variations in milling streams, studies on the impact of blending on the composition and rheological parameters of milling streams are limited. The published literature on blending

focuses on blending wheats of the same cultivars. For instance, (Dizlek & Özer, 2017) detailed how to improve the functionality of pest-damaged wheat by blending it with undamaged wheat of same variety; (Levent & Bilgiçli, 2017) blended wheats of the same cultivar harvested at different maturities. Moreover, the authors studied the effect of the blending ratio on the physicochemical and rheological characteristics of straight grade flour (i.e., a homogeneous mixture obtained by combining flour from all milling streams). Nevertheless, the influence of blending on the functionality of flour from different milling streams is often overlooked, as are the tempering conditions. Understanding the compositional variations in different milling streams as a function of blending and tempering would assist in optimizing the milling process of hard wheat, both in terms of quality and cost. Furthermore, the global market for bread is expected to increase to 135 million tons by 2025 (Statista, 2023). Subsequent rises are evident in the consumption and retail market price of bread (Statista, 2023). This necessitates further studies on hard wheat blending and its impact on flour functionality. Thus, the specific objective of this study was to understand the influence of blending different cultivars of wheat (i.e., hard red winter and hard red spring) on the composition, particle characteristics, and functionality of flour from different milling streams. Moreover, the impact of tempering conditions (i.e., moisture and time) on the chemical and rheological properties of flour from the blends were studied.

## **6.2 Materials and Methods**

### **6.2.1 Test Material**

The hard red winter (HRW) and hard red spring (HRS) wheat grains used in the study is procured from Montana Flour and Grain (Fort Benton, Montana, USA). The moisture contents of the grains were measured following ASABE standard S352.2 for whole kernels using the oven

method (ANSI/ASABE, 2012); protein contents were assessed through the AACC 46-30.01 protocol (AACC International, 2011). The moisture and protein contents of the HRW wheat grain were 13.2% (w.b) and 10.5%, respectively, whereas those of the HRS wheat grains were 11.7% (w.b) and 16.5%, respectively.

### **6.2.2 Milling**

Initially, the wheat samples (HRW and HRS) were tempered under the studied conditions i.e., tempering time of 16, 20, 24h and moisture content of 14%, 16%, and 18%). Thereafter, the tempered HRW and HRS wheat samples were mixed in different ratios to obtain blends (2000g) of varying protein content. These blends were milled using laboratory mill (Model: MLU 202, Make: Buhler Bros, Switzerland) according to AACC 26-21.02 (AACC International, 2011). The three different blends used in the study were B1 (25% HRW: 75% HRS), B2 (50% HRW: 50% HRS), and B3 (75% HRW: 25% HRS). After milling, the flour from three break rolls (1 BK, 2 BK and 3 BK) and reduction rolls (1 M, 2 M and 3 M) was collected separately for all wheat samples (Figure 6.1). Furthermore, the straight grade flour was prepared by recombining the flour from all the streams. For the experiments, all other milling parameters including roll gap and roll differential were kept constant.

### **6.2.3 Compositional analysis**

The chemical composition of the flour streams and straight grade flour was determined according to standard protocols: crude protein (AACC 46-30.01), ash (AACC 08-01.01), moisture content (AACC 44-15.02), and damaged starch (AACC 76-33.01) (AACC International, 2011). The amperometric method of damage starch analysis using SDmatic (Model: SDmatic, Make: Chopin technologies, Villeneuve-la-Garenne, France) is based on the absorption of iodine by damaged starch. Briefly, a solution was prepared by adding 120 mL of

distilled water containing 3 g of potassium iodide (KI), 1.5 g of citric acid ( $C_6H_8O_7$ ), and 1 drop of sodium thiosulphate ( $Na_2O_3S_2$ ). After the solution in the reaction bowl reached 35 °C, 1 g of flour was dispersed into the solution. The absorption of iodine by starch varies with the intensity of the damage and is measured.

#### **6.2.4 Particle size analysis**

The particle analyzer Malvern Morphology G3 (Model: G3, Make: Malvern Panalytical, Grovewood Road, UK) was used to determine the size distribution of the flour samples. The flour sample (5 mm<sup>3</sup>) was transferred to the dispersion chamber of particle size analyzer, where it was dispersed as a thin layer on the glass slide (Pezzali et al., 2020). Subsequently, the equipment analyzed the size characteristics of 5000 particles in a predefined area within the dispersion (Saad et al., 2011). Size distribution parameters obtained from the measurement included *d10*, *d50*, and *d90*. The values designated as *d10*, *d50* and *d90* indicate that 10, 50 and 90% of the measured particles are smaller than their respective value. It should be noted that all these diameters were calculated based on the assumption that the particles are spherical.

#### **6.2.5 Thermomechanical characteristics**

The variations in the consistency of dough when subjected to mixing with gradual increase in temperature were measured by the instrument Mixolab. Mixolab analysis has the potential to simultaneously assess the rheological properties and the viscoamylograph characteristics of dough subjected to heating and cooling cycles (viscoamylograph measurements are comparable to measurements from the rapid visco analyzer) (Espinosa-ramírez et al., 2021). Moreover, the equipment measures the water absorption capacity, dough stability during mixing, gelatinization characteristics and retrogradation of starch in a single analysis (Dubat, 2013a). Accordingly, the rheological behavior of dough as a function of mixing and temperature was studied following

AACC 54-60.01 (AACC International, 2011)- using Mixolab (Model: Mixolab, Make: Chopin Technologies, Villeneuve-la-Garenne, France). As per the protocol, initially, the dough was held at 30 °C for 8 min in the equipment mixer (Figure 6. 2). In the next stage the dough temperature was increased to 90 °C and maintained at that for 8 min. This stage enables gelatinization of starch granules. Furthermore, the temperature was reduced to 50 °C to simulate starch retrogradation. The experiments evaluated protein properties related to stability, elasticity and weakening. Starch gelatinization and retrogradation as affected by mixing and temperature were also monitored. The parameters measured during the Mixolab analysis are C1: initial consistency or torque during mixing at 30 °C (Nm), C2: Minimum torque (Nm) representing protein weakening, C3: peak torque experienced upon heating corresponding to starch gelatinization, C4: minimum torque during the heating phase representing gel stability, C5: torque during the cooling stage at 50 °C (Nm) corresponding to starch retrogradation during the cooling phase. The slopes  $\alpha$ ,  $\beta$  and  $\gamma$  measure the protein breakdown rate under the influence of heat, rate of gelatinization, and cooking stability rate, respectively. Apart from the primary parameters measured from the Mixolab analysis, the derived parameters evaluated include protein weakening range (C2–C1), pasting range (C3–C2), cooking stability (C4–C3), cooling setback (C5–C4), and pasting temperature range (D3–D2). Additionally, it measures the dough development time, i.e., the time to reach 1.1 Nm torque, the targeted consistency for bread dough (T1 in minutes) and the mixing resistance of the dough, represented as stability (DS in minutes). It should be noted that the flour yield from 3 BK was insufficient for Mixolab analysis and was excluded for all treatment combinations.

### 6.2.6 Statistical analysis

The effect of tempering time, moisture, samples, and fraction was assessed with a fixed effects model, as described by (Cappelli et al., 2020) using SAS Studio (SAS Institute Inc., Cary, USA). Analysis of variance (ANOVA) was used to test the significant differences in chemical and rheological qualities of the obtained flour. Homogeneity of variances was analyzed using the Levene test. The Tukey's test was performed following ANOVA to compare the means at a significance level of 5%. Principal component analysis (PCA) was applied to the data for pattern recognition. The data consisted of 5 rows (wheat)  $\times$  14 columns (quality indicators) for the samples. In the PCA, the number of components to be retained was determined based on the eigen values (one criterion) or Kaiser criterion.

## 6.3 Results

### 6.3.1 Flour yield

In the study, HRW wheat samples had higher milling yield (73.2%) compared with HRS (68.4%). Additionally, incorporation of greater percentages of HRS in the blend decreased the milling yield. For instance, B1, B2, and B3 had flour yields of 74.3%, 73.3%, and 72.9%, respectively (Table 6.1). It should be noted that though there was a reduction in - flour yield with increase in HRS content, the decrease was not statistically significant ( $p > 0.05$ ). However, in commercial milling, profitability is largely dependent on extraction. Thus, while not statistically significant, depending on the capacity of mills, even a 0.5% increase or decrease in the flour yield over time can influence the commercial value. Furthermore, varying the tempering moisture content from 14% to 18% resulted in an increase in flour yield from 71.7% to 73.1%. On the other hand, longer tempering time significantly ( $p < 0.05$ ) reduced the flour yield. For

instance, yield as high as 73.7% was obtained by tempering the grains for 16 h, while it was reduced to 70.6% at 24 h (Tables S4 and S5).

### **6.3.2 Compositional analysis**

Protein, ash, and damaged starch content of the flour samples varied with respect to the milling stream and tempering conditions. The influence of blending was more prominent on the protein content of the flour (Tables 6.1 and 6.2) than on ash and damaged starch. Increasing HRS content in the blend has varied the protein content of B1, B2 and B3 to 10.3, 11.4 and 12.9%, respectively (Table 6.1). Additionally, there was a significant increase in the protein content ( $p < 0.05$ ) with successive passages in the break stream. It varied from 13.41% in 1 BK to 16.75% in 3 BK. Tempering conditions also significantly ( $p < 0.05$ ) affected the protein content of milling streams (Table 6.2). As reported by (Warechowska et al., 2016), in this study, increasing the tempering moisture content reduced the protein content of the analyzed flour. Similar variations were also observed in the ash content of the flour. The ash content increased from 0.47% to 1.16% in the reduction streams ( $p < 0.05$ ). Similar increase in ash content of reduction streams were reported by (Sakhare & Inamdar, 2014). Apart from the milling streams, blending and tempering time significantly affected the ash content of the flour. Tempering the wheat for shorter duration (16 h) decreased the ash content to 0.47%. Though tempering time had a greater influence than moisture on the ash content (Table 6.2), tempering moisture also significantly affected the ash content of flour. The ash content was lowest (0.49%) when samples were tempered to 18% whereas it increased to 0.52% and 0.51% when the moisture was 14% and 16% (Tables S4 and S5).

The degree of starch damage varied significantly ( $p < 0.05$ ) in the milling streams (Table S6). In the break stream, the damaged starch content varied from 4.97% to 6.13%; and in the reduction

stream damage starch as high as 14.73% was observed. In the reduction streams of the mill, the degree of crushing is higher due to a smaller roll gap, resulting in finer flour with higher damaged starch. Increasing the tempering moisture from 14 % to 18% resulted in an increase in the damaged starch content from 8.7% to 9.5%. When increasing the tempering time from 16 to 24 hours, the damaged starch content decreased from 9.37% to 8.83%. Although there was a decrease in the damaged starch content, the reduction was not statistically significant ( $p > 0.05$ ). ANOVA results showed that the interaction between moisture content and time had a significant impact on the damaged starch content of the flours (Table 6.2). Additionally, the data for damaged starch showed that tempering time influences the variations in break flour streams, whereas tempering moisture has a prominent impact in reduction streams. Higher percentages of HRS in the blends increased the damaged starch content of the flour (Table 6.1) though the differences were not statistically significant ( $p > 0.05$ ). Moreover, ANOVA results showed that milling streams (fraction) and tempering conditions significantly contributed to the variation in damaged starch, rather than blending.

### **6.3.3 Particle size analysis**

Particle characteristics of flour were represented by d10, d50 and d90 values. Differences in grain hardness between HRW and HRS samples contributed to variations in the d10, d50 and d90 values of the samples. For example, the d10 values for HRW and HRS were 22.6  $\mu\text{m}$  and 25.4  $\mu\text{m}$ , respectively. Blending significantly influenced the particle characteristics of flour (Tables 6.1 and 6.2). Additionally, differences in the diameters were observed among the mill streams (fractions). For instance, d10, d50, and d90 for flour from 1 BK were 40.7, 96.6, and 166.8  $\mu\text{m}$ , respectively whereas it was 20.1, 60.7, 122.7  $\mu\text{m}$ , respectively for the flour obtained from 3 M. Differences in operational parameters like roll gap and roll differential influenced the

particle size distribution of the milling streams. While there were significant ( $p < 0.05$ ) changes in the d10 value with respect to tempering moisture (Table S4), the d50 and d90 were not significantly ( $p > 0.05$ ) affected by tempering conditions. Apart from blending and moisture content, the interactions between wheat  $\times$  tempering time and moisture content  $\times$  tempering time also contributed to the variations in particle characteristics such as d10, d50, and d90 (Table 6.2).

### **6.3.4 Thermomechanical analysis**

The rheological behavior of wheat dough is influenced by water, starch, and protein. In addition to its major components, other minor constituents like pentosans and enzymes contribute to the complex rheological characteristics of the flour. When wheat flour is mixed with sufficient water, solubilization and unfolding of the protein occur, and it forms a continuous network. The starch molecules are embedded into this protein network to form viscoelastic dough. The viscoelastic characteristics of dough undergo changes during mixing and heating. Mixolab measures the changes in the dough system pertaining to simultaneous heating and mixing. Water absorption (WA) is the amount of water required for the samples to reach an initial torque of 1.1 Nm (at 30 °C) for dough development. In the analysis, WA varied with respect to samples and milling stream. HRS samples had the highest WA of 68.8%. WA increased from 58.3% to 72.2% as the samples varied from 1 BK to 3 M. Even though grain moistening to 18% and longer tempering duration (24 h) increased the WA, the changes were statistically not significant ( $p > 0.05$ ).

The C1 scores of the Mixolab analysis (corresponding to dough development at 30 °C) were statistically similar with respect to tempering conditions, sample, and milling streams. Although there was a gradual increase in the values with an increase in the protein content of the flour for the blends, the increase was statistically insignificant ( $p > 0.05$ ). T1 is the time required by the

equipment to reach the required consistency of 1.1 Nm. T1 for the flour was higher (155.29 s) when the grains were tempered to 14% moisture content compared to 18% (135.75 s) (Table 6.3). Stability (DS) represents the time for which the torque of the dough stayed above 1.1 Nm during the initial mixing phase, and it varied from 6.9 min to 9.3 min for different samples. It also varied significantly ( $p < 0.05$ ) with the milling stream. For instance, DS decreased from 10.1 min (1 BK) to 8.2 min for 3 M. Although there was an increase in the dough stability with grain moistening and tempering time, the increase was statistically insignificant ( $p > 0.05$ ).

Increasing the temperature of the system to 60 °C weakens the proteins and initiates the gelatinization of dough. The low energy hydrogen bonds in the glutenin network are easily broken with increase in the temperature (Dubat, 2013a). Thus, in the second phase of the Mixolab analysis, the torque value (C2) decreases. There was a significant increase in the C2 value with an increase in tempering moisture content. C2 values also decreased with flour from successive milling streams (0.48 to 0.38). The protein weakening temperature (D2) varied among the samples. The weakening temperature was 55 °C for HRS whereas it was 53.6 °C for HRW (Table 6.3). The protein of the break flour streams had comparatively higher thermal stability (55.3 °C) than those from the reduction streams (~54 °C). Additionally, tempering the grains to 18% decreased the thermal stability (with mixing) to 53.5 °C than at 14% (55 °C). Furthermore, the protein breakdown rate ( $\alpha$ ) was statistically similar for all the test conditions. Tempering conditions and blending did not significantly vary the protein breakdown rate.

In the third stage of testing, the C3 scores (indicating starch gelatinization and pasting) decreased with blending. The decrease was proportional to the increase in HRS content. Among the samples, the lowest C3 value was observed for the HRS wheat (0.9 Nm). Tempering conditions did not significantly ( $p > 0.05$ ) influence the starch gelatinization and pasting characteristics (C3

values). Flour from the reduction streams had significantly lower C3 compared with break streams. Additionally, for break streams, C3 values were as high as 1.5 Nm, whereas it was successively reduced to 1.3, 1.1, and 0.8 Nm with passage from 1 M to 3 M. The rate of gelatinization ( $\beta$ ) was statistically different among the samples (Table 6.3). For example,  $\beta$  varied from 0.09 (HRS) to 0.21 (HRW). Tempering conditions had a negligible influence on the rate of gelatinization.

In the last stage of analysis, Mixolab measures gel stability (C4), i.e., soundness of starch fraction of the flour. It also corresponds to the presence of amylases in the samples. Though the variation was not significant ( $p > 0.05$ ), C4 varied with respect to the wheat samples (ranging from 1.4 to 1.7 Nm). Additionally, C4 values varied greatly among the milling streams. C4 was 1.8 Nm for 1 BK, whereas it was reduced to 1.2 Nm for 3 M. The cooking stability rate ( $\gamma$ ) of the analyzed samples was not influenced by blending and tempering conditions. The torque obtained at the end of the test (C5) varied significantly ( $p < 0.05$ ) with respect to the samples. The final torque was 2.6 Nm for B1 and decreased to 1.9 Nm for HRS samples. The flour samples exhibited a decrease in the final torque with an increase in protein content. Even though the break streams had higher torque compared with the reduction streams, there was a significant reduction in C5 torque with successive milling streams.

The blending and tempering moisture had a significant ( $p < 0.05$ ) influence on the pasting temperature range (D3–D2), which is the difference between protein weakening temperature and the temperature at C3. For instance, it increased from 14.71 °C for samples tempered to 14% (w.b) to 17.84 °C for 18% (w.b). Increasing the proportion of HRS content significantly ( $p < 0.05$ ) narrowed the pasting temperature range (Table 6.3).

### 6.3.5 Principal component analysis (PCA)

PCA was performed to understand the quality variation among the blended samples and their interrelationships. In the process, the original variables were compressed to two principal components (Eigen value greater than 1). This enables the identification of similarities and differences based on the correlation of variables and pattern recognition. In the analysis, 92.29% variability in the data was explained by the first two PC's, where 77.5% of variability was explained by PC1 and 14.8% by PC2 (Figure 6.2). In a PCA plots, variables appearing close to each other represent positive correlation whereas, those in the opposite directions indicate negative correlations. Upon analyzing the PCA biplot, it was noticed that an increase in WA was positively correlated with protein content ( $r = 0.95$ ), ash content ( $r = 0.35$ ) and particle characteristics than damaged starch. The damaged starch content influenced C3, C4, and C5 ( $r = 0.58, 0.58$  and  $0.87$ , respectively) values of flour. Dough stability (DS) ( $r = 0.2$ ) and pasting temperature range (D3–D2) ( $r = 0.57$ ) were positively correlated with damaged starch, while negatively correlated with protein content ( $r = -0.81$  and  $-0.90$ , respectively). Additionally, a positive correlation between protein and protein weakening temperature (D2) ( $r = 0.95$ ) as well as WA ( $r = 0.95$ ) was observed. As expected, the blend B2 (with 50% HRW and HRS) had rheological characteristics in between the control samples (Figure 6.3). Rheological characteristics, especially starch gelatinization and pasting, gel stability and final viscosity were mostly determined the similarity of B1 with HRW.

## 6.4 Discussion

### 6.4.1 Compositional analysis

In the analysis, there was an increase in the protein and damaged starch content of the flour with milling stream and blends. It was observed that the increase in the protein content was prominent in the break stream, while the damaged starch content varied greatly in the reduction streams.

This can be associated with the differences in the protein distribution inside the wheat kernels. In a typical wheat grain, the proportion of protein in the mature endosperm increases radially towards the outward direction (Tosi et al., 2011). This differential distribution of the protein inside the kernel, the presence of peripheral endosperm and the inclusion of finer bran particles rich in protein (Pojić et al., 2014) contribute to the increase in protein content of the flour in the break streams. Along with the protein content, the protein composition also varies throughout the wheat kernel, contributing to variability in functional properties. Thus, flour from the central endosperm has better functional properties, even though it has lower protein content (Yahata et al., 2006). There was a higher percentage of ash content in the tail end streams (Sakhare & Inamdar, 2014) as the final milling streams receive relatively bran rich tail end flour from the 3 BK. Furthermore, at lower moistures, the kernels are brittle, resulting in finer bran fractions in the flour, which contribute to higher ash content.

Mechanical damage of starch is inevitable in the milling of grains (Q. Wang et al., 2020). Shear forces during roller milling of wheat causes crystalline damage in the starch—protein interface, resulting in mechanical damage of the starch (Ma et al., 2020). The extent of damage is influenced by the kernel characteristics (hardness) and mill operational parameters (roll gap, roll speed, roll differential). Furthermore, milling intensity increases in the reduction streams with a reduced roll gap, resulting in finer flour fractions. As the flour fineness increases, the degree of

starch damage also increases (Barak et al., 2014; Monnet et al., 2019; Siliveru et al., 2017).

Tempering conditions also influence the composition of the flour (Warechowska et al., 2016).

Tempering, or grain moistening, results in the development of cracks in the endosperm (Woźniak & Styk, 1996). The plane of these cracks intersects transversely with the starch granules (Warechowska et al., 2016). This increases the chances of mechanical damage to starch with an increase in tempering moisture (Ghodke et al., 2009).

#### **6.4.2 Particle size**

Particle size distribution of the flour depends on factors such as tempering, roll adjustments and wheat characteristics (Posner et al., 2014). As expected, the particle size of the flour varied with respect to the tempering conditions. Higher mean particle sizes were observed when tempering grains to 18% (Cappelli et al., 2020; Warechowska et al., 2016). In the study, tempering time did not impact the d10 values as the studied time (greater than 16 h) was significant enough to ensure the moisture migration inside the kernels. Moreover, there was an increase in mean particle size of the flour with an increase in the proportion of HRS in the blend. With higher proportion of HRS, the overall hardness of wheat kernels increased resulting in larger flour particles (Patwa et al., 2014). The particle size of the flour significantly influenced the physicochemical and functional properties of wheat flour (Pang et al., 2021).

#### **6.4.3 Thermomechanical properties**

The WA of the flour depends on the quality and content of proteins, the native starch and damaged starch content, and the fiber (pentosans) content (Dubat, 2013a). In the study, the protein content varied among the samples and was the prominent contributor to the WA (Figure 3). A higher percentage of HRS concurrently increased the WA due to the greater content of

gliadins and glutenins (Maghirang et al., 2006). Moreover, the increases were consistent with the observations of (Sluimer, 2005)(Table 6.3). According to the empirical method proposed by Sluimer (Sluimer, 2005), WA is expected to increase by 1% (w/w) for every 1% increase in protein content (Dubat, 2013a). Additionally, the proportion of B-type granules is higher in the HRS wheat (Park et al., 2009), and these granules have a higher affinity for water than A-type granules at room temperature (Chiotelli & Meste, n.d.) increasing the WA with HRS content in the samples.

During the mixing stage, hydration of proteins leads to their expansion. This increases the interaction between the thiol groups of the protein, and disulfide bonds are created, which plays a significant role in formation of the gluten network. Furthermore, the starch granules are embedded in the gluten network forming the dough. Thus, behavior of the dough is also dependent on the starch content. Increasing the temperature from 30 to 90 °C during the analysis weakens the protein network and gelatinizes the starch. Unlike in batter, where complete gelatinization of starch occurs upon heating, in dough systems, gelatinization of starch is incomplete due to the limited availability of water. It leads to the transfer of moisture from proteins to starch during cooking (Dubat, 2013a). These changes in the protein and starch during mixing and cooking depends on the composition of starch (A- and B-type granules) (Park et al., 2009) and protein (gliadin, glutenin, polymeric proteins) (Maghirang et al., 2006), temperature and water activity (Hoseney et al., 1978). The observed differences in the Mixolab parameters (torque C2 to C5) of the samples can be attributed to these compositional differences in HRW and HRS.

The distribution of lipids (Prabhasankar & Haridas Rao, 2001), fatty acids (Prabhasankar et al., 2000), free amino acids and sulfur (Liu et al., 2011), free thiol groups (Menkovska et al., 2002),

disulfide linkages (Ma et al., 2020) and enzymes (Rani et al., 2001) varies among the mill streams. Additionally, there is variable distribution of protein concentration and composition (Pojić et al., 2014; Y. G. Wang et al., 2007) among different mill streams, contributing to differences in the rheological properties. The concentration of polymeric protein in relation to monomeric protein is greater in break streams than in the reduction streams (Y. G. Wang et al., 2007), resulting in a lower degree of disulfide cross linking (Pojić et al., 2014; Y. G. Wang et al., 2007). These differences result in higher C2 values of the break flour streams than in the reduction streams. Furthermore, reduction streams have higher  $\alpha$ -amylase content (Rani et al., 2001) and damaged starch. It is reported that damaged starch is prone to hydrolysis by  $\alpha$ -amylase (Hoseney, 1994). The concomitant increase in the enzyme and damaged starch is associated with a decrease in C3, C4 and C5 torques (Codină et al., 2019) in the reduction streams. Moreover, the activity of the enzyme leads to the production of dextrans, which in turn impacts the water holding capacity and porosity of the dough (Barrera et al., 2007). The difference in these distributions corresponds to variability in the rheological properties among milling streams.

The PCA analysis exhibited a negative correlation between particle characteristics and damaged starch. This inverse relationship implies that a reduction in particle size is associated with an increase in starch damage, which in turn is positively correlated with WA. Moreover, a reduction in particle size promotes redox conversion of sulfhydryl (-SH) groups to disulfide group (Ma et al., 2020). This leads to the cross linking of low molecular weight gluten to form high molecular weight glutenin subunits, thereby increasing the gluten macro molecular protein content (Ma et al., 2020). Ash content also influences the WA. This is attributed to the higher water binding capacity of arabinoxylans present in the aleurone layer and bran. Thus, the particle

characteristics, ash, and protein content interfere with the water absorption characteristics (Pojić et al., 2014). Damaged starch has influenced the gelatinization and pasting properties of the dough (Hackenberg et al., 2019). An increase in gliadin content with incorporation of HRS in the blends decreases the stability of the dough (Barak et al., 2014; Maghirang et al., 2006). This results in a negative correlation between protein content and dough stability.

By blending HRS and HRW, the protein content was intentionally varied, contributing to a change in the quality of protein among the samples. Subsequent changes in the starch granule type and distribution also occur in the blends (Park et al., 2009). These differences contribute to changes in WA and other rheological properties of the dough. From the PCA analysis, it is evident that the WA characteristics were closely associated with protein content rather than the damaged starch. Thus, in blends with a higher proportion of HRS, the protein content is the primary determinant of particle characteristics, WA, and pasting temperature.

## **6.5 Conclusions**

In summary, tempering and blending affected the composition and particle characteristics of flour. These variables had a significant influence on particle size, damaged starch content, and protein content; subsequent differences were observed in the rheological properties. Flour from break and reduction streams differed in composition and rheological properties contributing to the differences in functionality. Variations in the properties were also exhibited by successive milling streams in both break and reduction passages. An increased proportion of HRS in the blends varied the pasting characteristics and cooking stability of the flour. The experiments illustrated that blending not only affects the protein content and composition but also the starch quality and thus the rheological properties. Therefore, tempering and blending can effectively modify the rheological and functional properties of flour.



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## Tables

**Table 6.1. Effect of hard wheat blending on flour yield, particle characteristics and chemical properties of straight grade wheat flour**

|        | Flour Yield              | <i>d</i> 10                | <i>d</i> 50               | <i>d</i> 90                | Protein                    | Damaged Starch           | Ash                      |
|--------|--------------------------|----------------------------|---------------------------|----------------------------|----------------------------|--------------------------|--------------------------|
| Sample | (%)                      | (µm)                       | (µm)                      | (µm)                       | (%)                        | (%)                      | (%)                      |
| HRW    | 73.22 (3.6) <sup>A</sup> | 22.61 (0.96) <sup>B</sup>  | 69.03 (10.1) <sup>A</sup> | 131.82 (17.9) <sup>A</sup> | 9.41 (0.42) <sup>D</sup>   | 9.25 (2.32) <sup>A</sup> | 0.55 (0.12) <sup>A</sup> |
| B1     | 74.33 (2.9) <sup>A</sup> | 23.43 (2.55) <sup>AB</sup> | 74.24 (13.4) <sup>A</sup> | 130.14 (20.6) <sup>A</sup> | 10.28 (0.66) <sup>CD</sup> | 8.37 (1.26) <sup>A</sup> | 0.44 (0.11) <sup>A</sup> |
| B2     | 73.23 (2.7) <sup>A</sup> | 24.09 (1.80) <sup>AB</sup> | 75.09 (7.1) <sup>A</sup>  | 141.01 (13.8) <sup>A</sup> | 11.39 (1.11) <sup>C</sup>  | 9.51 (1.89) <sup>A</sup> | 0.44 (0.21) <sup>A</sup> |
| B3     | 72.88 (1.9) <sup>A</sup> | 24.00 (2.30) <sup>AB</sup> | 77.76 (6.6) <sup>A</sup>  | 129.99 (7.7) <sup>A</sup>  | 12.94 (1.43) <sup>B</sup>  | 9.08 (2.03) <sup>A</sup> | 0.43 (0.18) <sup>A</sup> |
| HRS    | 68.38 (7.6) <sup>A</sup> | 25.44 (3.01) <sup>A</sup>  | 79.55 (9.9) <sup>A</sup>  | 143.02 (10.0) <sup>A</sup> | 15.88 (0.69) <sup>A</sup>  | 8.63 (2.32) <sup>A</sup> | 0.60 (0.20) <sup>A</sup> |

**Table 6.2. Percent variance components across dataset for physicochemical characteristics as function of wheat, moisture content (MC), tempering time, milling stream and their interactions**

| Source                        | Damaged Starch | Ash   | Protein | <i>d10</i> | <i>d50</i> | <i>d90</i> |
|-------------------------------|----------------|-------|---------|------------|------------|------------|
| Wheat                         | 3.27           | 8.45  | 68.02   | 8.57       | 9.45       | 7.24       |
| Moisture content (MC)         | 4.63           | 2.1   | 0.38    | ns         | 3.15       | ns         |
| Time                          | 2.59           | 7.31  | 0.77    | ns         | ns         | ns         |
| Milling stream                | 78.79          | 67.65 | 27.25   | 85.95      | 71.22      | 73.35      |
| Wheat × MC                    | 0.88           | 4.61  | 0.88    | ns         | ns         | ns         |
| Wheat × Time                  | 1.67           | 1.22  | 0.41    | 0.99       | 1.87       | 2.78       |
| Wheat × Milling stream        | ns             | ns    | 0.57    | 0.74       | ns         | 2.34       |
| MC × Time                     | 5.95           | 4.64  | 0.60    | 2.71       | 7.71       | 7.23       |
| MC × Milling stream           | ns             | ns    | 0.25    | 1.04       | 1.82       | ns         |
| Time × Milling stream         | ns             | 1.12  | 0.20    | ns         | ns         | ns         |
| Wheat × MC × Time             | 1.85           | 2.91  | 0.50    | ns         | 1.49       | ns         |
| Wheat × MC × Milling stream   | ns             | ns    | ns      | ns         | 1.42       | 2.49       |
| Wheat × Time × Milling stream | ns             | ns    | 0.17    | ns         | ns         | 2.45       |
| MC × Time × Milling stream    | 0.38           | ns    | ns      | ns         | 1.87       | 2.12       |

ns: not significant

**Table 6.3. Effect of hard wheat blending on rheological properties of dough measured by Mixolab.**

| Rheological Properties | Samples                   |                             |                             |                            |                          |
|------------------------|---------------------------|-----------------------------|-----------------------------|----------------------------|--------------------------|
|                        | HRW                       | B1                          | B2                          | B3                         | HRS                      |
| WA (%)                 | 62.9 (6.4) <sup>B</sup>   | 61.5 (6.0) <sup>B</sup>     | 62.8 (3.4) <sup>B</sup>     | 65.9 (5.2) <sup>AB</sup>   | 68.9 (3.1) <sup>A</sup>  |
| C2 (Nm)                | 0.48 (0.05) <sup>A</sup>  | 0.46 (0.05) <sup>A</sup>    | 0.47 (0.04) <sup>A</sup>    | 0.45 (0.05) <sup>A</sup>   | 0.4 (0.04) <sup>B</sup>  |
| C3 (Nm)                | 1.5 (0.5) <sup>A</sup>    | 1.5 (0.5) <sup>A</sup>      | 1.3 (0.4) <sup>A</sup>      | 1.2 (0.4) <sup>AB</sup>    | 0.9 (0.3) <sup>B</sup>   |
| C4 (Nm)                | 1.6 (0.3) <sup>A</sup>    | 1.6 (0.3) <sup>A</sup>      | 1.7 (0.4) <sup>A</sup>      | 1.4 (0.5) <sup>A</sup>     | 1.4 (0.2) <sup>A</sup>   |
| C5 (Nm)                | 2.5 (0.6) <sup>A</sup>    | 2.6 (0.5) <sup>A</sup>      | 2.5 (0.3) <sup>A</sup>      | 2.2 (0.5) <sup>AB</sup>    | 1.9 (0.3) <sup>B</sup>   |
| $\alpha$               | -0.08 (0.0) <sup>A</sup>  | -0.11 (0.2) <sup>A</sup>    | -0.08 (0.0) <sup>A</sup>    | -0.07 (0.0) <sup>A</sup>   | -0.08 (0.0) <sup>A</sup> |
| $\beta$                | 0.21 (0.1) <sup>A</sup>   | 0.14 (0.1) <sup>AB</sup>    | 0.15 (0.1) <sup>AB</sup>    | 0.12 (0.1) <sup>B</sup>    | 0.09 (0.1) <sup>B</sup>  |
| $\gamma$               | -0.03 (0.1) <sup>AB</sup> | -0.06(0.1) <sup>B</sup>     | 0.02 (0.1) <sup>A</sup>     | -0.02 (0.1) <sup>AB</sup>  | 0.03 (0.1) <sup>A</sup>  |
| C2-C1 (Nm)             | -0.63 (0.0) <sup>A</sup>  | -0.64 (0.1) <sup>A</sup>    | -0.65 (0.0) <sup>A</sup>    | -0.61 (0.2) <sup>A</sup>   | -0.71 (0.0) <sup>B</sup> |
| C3-C2 (Nm)             | 0.96 (0.5) <sup>A</sup>   | 1.04 (0.1) <sup>A</sup>     | 0.8 (0.4) <sup>AB</sup>     | 0.82 (0.3) <sup>AB</sup>   | 0.51 (0.3) <sup>B</sup>  |
| C4-C3 (Nm)             | 0.1 (0.4) <sup>B</sup>    | 0.1 (0.5) <sup>B</sup>      | 0.4 (0.5) <sup>AB</sup>     | 0.2 (0.4) <sup>AB</sup>    | 0.5 (0.2) <sup>A</sup>   |
| C5-C4 (Nm)             | 0.91 (0.3) <sup>A</sup>   | 0.99 (0.5) <sup>A</sup>     | 0.8 (0.34) <sup>AB</sup>    | 0.77 (0.4) <sup>AB</sup>   | 0.55 (0.1) <sup>B</sup>  |
| T1 (s)                 | 66.68 (43.7) <sup>B</sup> | 146.2 (143.3) <sup>AB</sup> | 165.6 (135.6) <sup>AB</sup> | 212.1 (164.5) <sup>A</sup> | 184 (88.6) <sup>A</sup>  |
| Stability (min)        | 9.02 (0.7) <sup>B</sup>   | 9.91 (1.4) <sup>A</sup>     | 9.0 (1.0) <sup>B</sup>      | 8.86 (0.8) <sup>B</sup>    | 8.30 (0.8) <sup>B</sup>  |
| D2 (°C)                | 53.59 (2.0) <sup>B</sup>  | 54.02 (1.0) <sup>AB</sup>   | 54.43 (1.3) <sup>AB</sup>   | 54.82 (1.4) <sup>AB</sup>  | 55.03 (1.3) <sup>A</sup> |
| D3-D2 (°C)             | 19.59 (4.9) <sup>A</sup>  | 18.39 (5.3) <sup>AB</sup>   | 13.95 (4.3) <sup>C</sup>    | 14.21 (5.2) <sup>BC</sup>  | 12.87 (3.5) <sup>C</sup> |

Values are represented as mean ( $\pm$ standard deviation). Values designated by different letters in a row are significantly different at  $p = 0.05$ . HRW: Hard red winter, HRS: Hard red spring, B1: Blend 1 (25% HRS), B2: Blend 2 (50% HRS), B3: Blend 3 (75% HRS), WA: Water absorption, C1: Torque at mixing (30 °C), C2: Protein weakening, C3: Starch gelatinization, C4: Starch gelling, C5: Starch retrogradation,  $\alpha$ : protein breakdown rate,  $\beta$ : rate of gelatinization,  $\gamma$ : cooking stability rate, C2-C1: Protein weakening range, C3-C2: Pasting range, C4-C3: Cooking stability, C5-C4: Cooling setback, T1: Time to reach C1, DS: stability, D2: temperature at protein weakening, D3-D2: Pasting temperature range.

## Figures

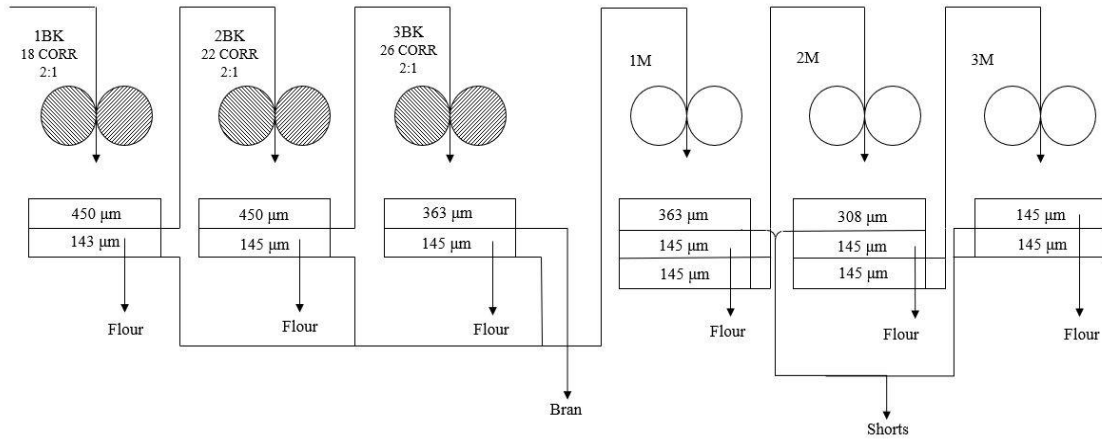


**Figure 6.1. Mill flow sheet of the laboratory mill (Buhler MLU-202). BK: Break roll, M: Reduction roll, CORR: corrugations per inch on the roll (e.g., 18 CORR-18 corrugations/inch), 2:1 is the roll differential.**

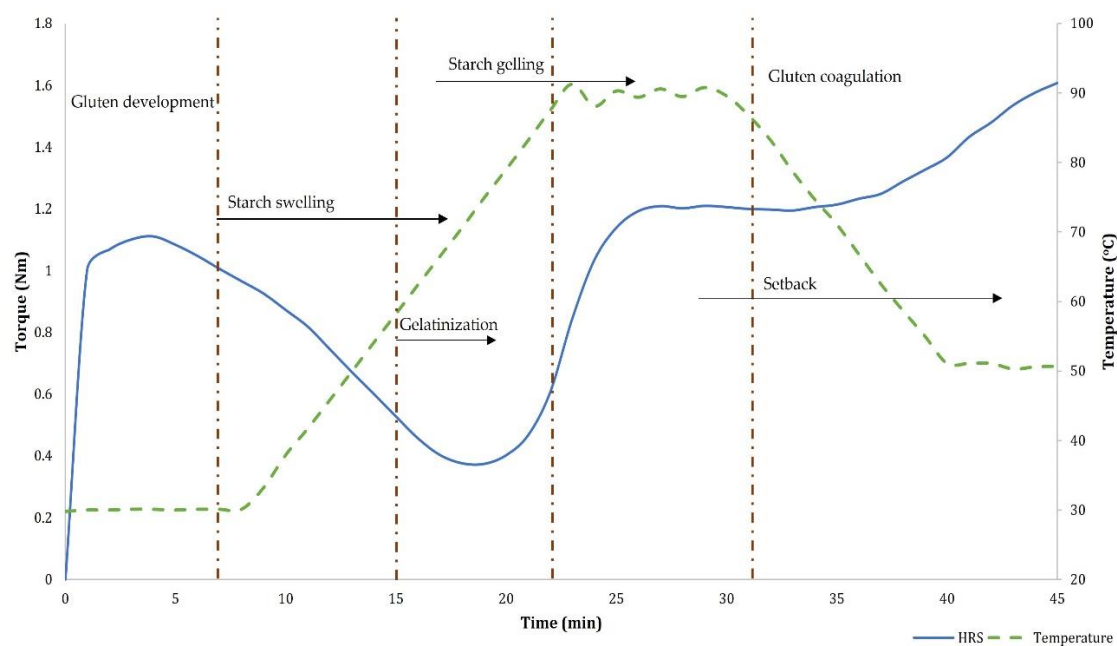


**Figure 6.2. Sample Mixolab profile representing the changes during the Mixolab analysis. The image was prepared by referring to (Dubat, 2013b)**

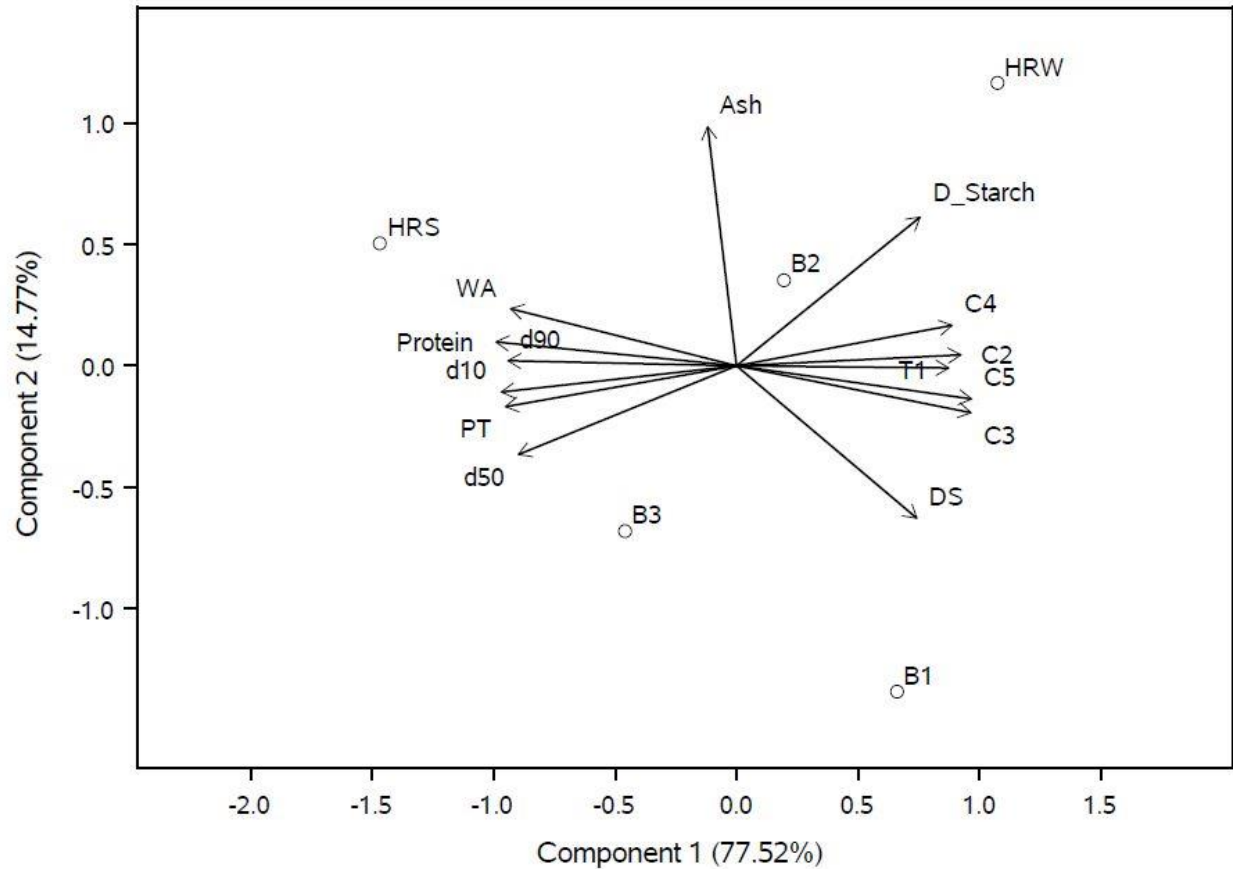


**Figure 6.3. PCA biplot (PC1 vs PC2) for physicochemical and rheological properties.** HRW: Hard red winter, HRS: Hard red spring, B1: Blend 1, B2: Blend 2, B3: Blend 3, D\_starch: damaged starch, WA: Water absorption, C2: Protein weakening, C3: Starch gelatinization, C4: Starch gelling, C5: Starch retrogradation, DS: Dough stability, D2: temperature at protein weakening, D3\_D2: Pasting temperature range.

## **Chapter 7 Predicting rheological properties of wheat dough from flour properties using NIR coupled with artificial neural network<sup>4</sup>**

### **Abstract**

Farinograph analysis serves as the standard for determining the baking quality of wheat flour. It measures water absorption (WA), dough development time (DDT), and stability (DS) of wheat dough. These characteristics depend on wheat flour properties such as protein content, moisture, ash, and falling number. Additionally, farinograph analysis is costly, time-consuming, and requires skilled personnel. Therefore, an artificial neural network (ANN) model was developed to predict the farinograph properties of wheat dough as a function of flour properties. The models were developed using data from 192 wheat samples. Multi-layer perceptron type feed-forward ANN models with increasing complexity were developed for each response variable, i.e., ANN-WA, ANN-DDT, and ANN-DS, and the model success was evaluated via mean squared error (MSE) and correlation coefficient ( $r$ ). The optimal models had two to four hidden layers, each with five to sixty neurons, and exhibited the lowest MSE and highest  $r$  values. In terms of predictive performance, the models ANN- WA and ANN- DDT ( $r = 0.79$ ) demonstrated superior performance when compared with ANN-DS ( $r = 0.63$ ). Feature importance analysis was conducted to provide insight on variable contributions, underscoring the significance of flour protein content in the model's prediction. The study explored the applicability of data-driven ANN models in predicting the rheological characteristics of dough. The developed models could

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<sup>4</sup> Submitted for publication: Journal of the ASABE

serve as a decision support tool and aid millers in adjusting mill settings and bakers in modifying the dough mixing based on dough rheology.

## **7.1 Introduction**

Wheat (*Triticum aestivum* L.), a staple food widely utilized in various baked goods such as bread, cakes, cookies, pasta, and snacks, is holding significant importance in the global food system. In 2020-2021, the global wheat production was 771 million metric tons (MMt), with the United States contributing 47.3 MMt, accounting for approximately 6% of the total global production (FAOSTAT, 2021). Kansas is the largest wheat producing state in the US (Raj et al., 2023), specializing in the cultivation of hard winter wheat primarily used to produce bread. Thus, the milling and baking quality of wheat plays a crucial role in the marketing of the grains to the primary purchasers: millers and bakers (Vitale et al., 2020).

Various parameters determine the end-use quality of wheat, including protein content, kernel weight, moisture content, gluten content, milling yield, falling number value, and rheological properties (Mutlu et al., 2011). Protein content is the primary quality component influencing the baking characteristics of wheat (Corassa et al., 2018; Koppel & Ingver, 2010). It serves as a reliable indicator of bread loaf volume and dough rheological properties (Park et al., 2006).

Another important parameter impacting flour's baking quality is amylase activity, which can be measured through falling number analysis (Hu et al., 2022). Amylase activity influences dough development time (Dencic et al., 2013) and consequently affects the mixing characteristics of the dough. Additionally, moisture content affects the water absorption of the flour, thereby producing a dough with a workable consistency.

Rheological properties provide valuable insights into flour quality, the mechanical behavior of dough during handling processes (e.g., mixing, dividing, rounding), textural characteristics of the final product, and processing efficiency (Abbasi & Seyedin, 2012). Conventionally, instruments such as farinograph, extensograph, alveograph, and mixograph are commonly employed to measure these properties (Mutlu et al., 2011). However, despite their reliability, these conventional techniques are associated with high costs, time-consuming procedures, and the requirement for skilled technicians. Therefore, the development of fast and reliable methods for determining the rheological quality of flour offers an opportunity to improve system's efficiency. Additionally, developing models to predict the rheological properties using simple measurable flour properties can help in online process control in milling industry and modifying the processing parameters (such as mixing time and speed) in bakeries. Because the development of high-yield, high-quality varieties by breeding entities also requires costly milling and baking evaluations, such advancements also hold potential for application in cultivar screening for grain quality within breeding programs.

Artificial neural networks (ANNs) imitate the biological nervous system to map nonlinear relationships between input and output. ANN based model offers flexibility, robustness, and adaptability to incorporate nonlinear mapping (Abbasi et al., 2014; Raj & Dash, 2020). This nonlinear computational modeling tool is used in a variety of applications, including food safety and quality analysis, as well as the modeling of numerous thermal and non-thermal operations (G. V. S. B. Raj & Dash, 2020a). Comprehensive review on the application of ANN in food (Ayed & Hanana, 2021; Raj & Dash, 2020a) provides a detailed overview on the available literature. These computational tools were effectively utilized for classification of oils and fruits (da Silva et al., 2015; Kumar & Durgesh, 2014), optimization of process parameters (Ameer et

al., 2017; Torrecilla et al., 2005), modeling the drying process (Betiku & Taiwo, 2015; da Silva Veloso et al., 2020; Raj & Dash, 2020b), prediction of extraction yield (Chokphoemphun & Chokphoemphun, 2018; Silveria et al., 2014), and real-time process control (Funes et al., 2015; Furferi et al., 2007). The potential of ANNs in predicting grain-related product characteristics are explored for varietal classification using morphological features (Dubey et al., 2006; Javanmardi et al., 2021; Kaya & Saritas, 2019), prediction of physical properties of flour (Fang et al., 1998) and various wheat quality parameters such as milling yield (Assadzadeh et al., 2021), noodle extensional properties (Kwon et al., 2022), pasting characteristics (Codină et al., 2019), dough rheology (Abbasi & Seyedin, 2012; Mutlu et al., 2011; Razmi-Rad et al., 2007) and more.

In the past decade, several ANN models were developed to predict the rheological properties of wheat flour (Abbasi et al., 2014; Mutlu et al., 2011; Razmi-rad et al., 2007). The feed forward multilayer perceptron (MLP) models developed by (Abbasi et al., 2014a; Razmi-Rad et al., 2007) to predict farinograph quality parameters relied on chemically analyzed flour properties (protein content, ash content, wet gluten content, gluten index, Zeleny sedimentation value, and falling number value) for their predictions. (Mutlu et al., 2011) investigated the potential of ANN to predict dough quality using near-infrared (NIR) spectra of flour. While these models have helped to identify parameters capable of predicting farinograph attributes, their predictability on unknown datasets is limited by the small datasets used for training and testing. Additionally, the rationale behind the predictions or how the models make decisions is often overlooked.

The NIR measurement of moisture content, protein content and ash content, as well as the analysis of falling number value, is fundamental during the wheat milling. These measurements impact purchasing decisions by millers (e.g., flour with a higher protein content in the range of 12 – 14 % is optimal for yeast leavened bread, while a lower protein content is preferred when

producing bread sticks). Moreover, these measurements influence the rheological properties of the wheat dough. In the present study, we propose an ANN to predict the rheological properties of dough based on the mentioned properties. The first goal is to develop a precise and effective ANN model to predict the farinograph properties of wheat dough as a function of flour properties, which would serve as a decision-making tool potentially for millers and bakers. While ANNs are considered as universal function approximators, capable of capturing complex non-linear input-output relationship, the ANN expressed relationship is not self-explanatory and often considered as a black box model. Therefore, the second goal of this study is to investigate the input-output relationship of the ANN model using variable contribution methods. Variable contribution, also known as feature importance, refers to the degree to which each input variable contributes to the ANN model prediction (Badgujar et al., 2022; Rodríguez-Perez & Bajorath, 2020b). This would address numerous inquiries regarding the rationale behind the network's predictions and facilitate the exploration of potential enhancements to elevate network performance (Badgujar et al., 2023).

## **7.2 Materials and Methods**

### **7.2.1 Wheat samples**

The study samples included different hard winter wheat varieties cultivated in Kansas, US, spanning the growing seasons between 2020-21 and 2021-22. Four wheat varieties (WB 4269, WB Grainfield, KS Dallas, and Zenda) were grown under four explicitly different management conditions in 24 environments across both seasons. The individual combination of environments, managements and varieties resulted in 192 scenarios used for assessing wheat milling and baking qualities. Here, each scenario is replicated in 3-8 field plots. Harvested wheat from the replicates is combined and milled in three separate replicates, and the resulting flour is analyzed for flour

properties and baking quality. Consequently, each scenario is the average of three milling and baking replicates. The farming practices and environmental conditions during the seasons are detailed in studies by Ryan and coauthors and beyond the scope of the current work (Ryan et al., 2022, 2023). The flour utilized for the analysis was obtained by milling wheat grains, which had been tempered to a moisture content of 15-16% over a 24 h period, following the protocol (AACC 26-21.02, 2009). Protein (AACC 39-11.01, 1999), moisture, and ash content (AACC 08-21.01, 2020) of the flour were measured using NIR spectrometer (Perten ® DA 7250, Perkin-Elmer Corp., Waltham, MA, US). The  $\alpha$ -amylase activity was determined through falling number analysis (AACC 56-81.04, 2019). A higher falling number value (FNV) correlates with lower enzyme ( $\alpha$ -amylase) activity and vice-versa.

Rheological characteristics of the flour were evaluated following the standard method, AACC 54-22.01 (AACC 54-22.01, 2011). As per the standard, the farinograph analysis evaluated water absorption (WA), dough development time (DDT), and dough stability (DS). Water absorption is defined as the quantity of water absorbed by the flour to develop a dough of 500 BU consistency. Dough development time (DDT) is the time (in minutes) elapsed between the addition of water and the development of peak consistency. Stability (expressed in minutes) is measured as the difference between the arrival time (farinogram first intercepts 500 BU line) and departure time (farinogram leaving 500 BU line).

### **7.2.2 Neural network model**

ANN architecture consists of multiple units called neurons, interconnected and organized in layers. A feedforward type of ANN comprises multiple connected layers with a uni-directional information flow, and a typical ANN architecture includes input, hidden, and output layers, as shown in Figure 7.1. A neuron is a basic functional unit, i.e., each neuron receives a numerical

input, performs a weighted computation, applies an activation function, and passes the output to the next layer (Raj & Dash, 2020a; Szwedziak & Wojtkiewicz, 2020). The activation function introduces nonlinearity into the network's output. The input and output layer size are determined by the number of input and output features, respectively. The intermediate layers are called hidden layers, allowing the network to learn and capture a complex and nonlinear relationship between input and output. The ANN models can include one or more hidden layers, each with several neurons depending upon the input-output complexity (Badgujar et al., 2022).

The ANN is trained on training data where network parameters (weights and biases) are adjusted iteratively to minimize the difference between the predicted and true outputs (Yu & Wilamowski, 2018). Training is an optimization process and involves: (1) forward propagation: a uni-direction information flow through the ANN to produce predictions, and (2) backward propagation: gradients are computed to update the neuron's parameters (weights and bias). The training continues until the network converges to a point where the network loss is reduced to an acceptable level or if there is no improvement in model performance.

In recent years, ANN has emerged as a powerful technique that excels at regression (predicting continuous numerical values) and classification problems (predicting class labels). One key advantage of ANN, particularly for regression, is their ability to handle highly nonlinear and complex patterns in the data (Badgujar et al., 2023; Zareef et al., 2020). Furthermore, the author's decision to use ANN over decision trees or random forests is driven by the possibility of incorporating additional data points into the training set, particularly as the study anticipates for additional samples from future harvesting seasons.

### **7.2.3 ANN model development**

The ANN model development is an iterative and multi-step process. The undertaken problem falls into a regression task in which the developed ANN models predict a continuous numerical value (dough characteristics) based on multiple input features (flour properties). In this study, independent ANN models were developed for each dough characteristics (WA, DDT, and DS) as a function of flour properties (Pro, MC, Ash and FNV) as an input, resulting in three ANN models. The models were developed in Python with the "Keras," an open-source software library used for implementing artificial neural networks (Manaswi, 2018). The steps involved in ANN regression model development are described in subsequent sections.

#### **7.2.3.1 Data processing**

Data processing is a standard operation, includes data cleaning, feature scaling, and reshaping performed prior to model development. Data cleaning was performed manually which included identifying missing values and outliers. Feature scaling ensures that all model features are on a similar scale. It helps the model to converge faster, improves training stability, and prevents certain features from dominating others. The common feature scaling technique called Z-score standardization was performed on inputs and output features. It transformed each feature with a mean zero and a standard deviation of one. Data reshaping transforms the data into a specific shape required for model training. The data was reshaped into a 2-D (dimensional) array, where each row represented a sample, and each column represented a feature. Finally, the data was divided into model development and model evaluation subsets (test) in the ratio of 90:10. This resulted in 172 observations in the model development subset and 20 observations in the test set. The model development subset was further divided into train (80%) and validation (20%) subsets. The training subset was used for ANN model training and validation subset optimized

the model parameters. The test subset evaluated the final model and provided an unbiased estimate.

#### **7.2.3.2 ANN model architecture**

A multi-layered, feedforward ANN architecture was implemented (Fig. 7.1) and defined using a sequential model, that is a simple and intuitive method of building ANN in Keras (Chollet, 2015). The sequential model consisted of a linear stack of ANN layers that carry information in a sequential flow from input to output. The ANN models with multiple fully connected layers with varying neurons were developed. The number of input and output features determined the first and final layer size, respectively. An independent ANN model was developed to predict each dough characteristic (WA, DDT, and DS); hence, the output layer included a single neuron. Similarly, the input layer size included the flour properties i.e., four neurons in input layer (Fig. 7.1). The intermediate hidden layer size and number of neurons were determined based on data complexity and the model's ability to learn from the available data. The hidden layer (size and number) was manually updated by observing the model performance (loss i.e., MSE and  $r$ ) on the train and validation subset. The activation function accompanied each ANN layer. The Rectified Linear Unit (ReLU) nonlinear activation function was selected for a hidden layer to introduce the nonlinearity. The linear activation function was selected in the output layer, commonly used in regression tasks.

An optimizer and loss function determine how the ANN model is trained and optimized to make predictions. The Adaptive Moment Estimation (Adam) optimizer was selected to update the ANN parameters during training to minimize the loss function. The loss function quantified the difference between the model predicted and actual values. During training, loss function measured model performance and guided the optimization process. The loss function commonly

used in regression task called “Mean squared error (MSE)” was selected which computed the average squared differences between predicted and actual values.

### **7.2.3.3 Model training and evaluation**

The ANN training is an iterative process; therefore, a flowchart of model development and training was used as shown in Figure 7.2. The model training included the following steps: (1) Initially, the data was pre-processed and divided into model development and evaluation subset. (2) The ANN parameters such as learning rate, training epochs, and regularization methods were selected. Additionally, ANN architecture with two hidden layers were selected, and model parameters (weights and biases) were initiated randomly. (3) The model training was initiated for 1000 epochs, where the input features were fed to the model and forward passed, the loss (MSE) was computed on train and validation subset for each epoch while updating the model parameters through gradient backpropagation (Adam optimizer) method. (4) The model learning curves (train and validation subset loss or MSE) were monitored. (5) The regularization method called early stopping was implemented, where the learning curves (train and validation loss) were monitored, and training was stopped if the validation loss did not improve for a predefined number of epochs (60 epochs) or model performance started to degrade i.e., validation loss starting to increase after reaching to the lowest. (6) The trained ANN model was evaluated on both model development and evaluation subset on matrices specific to regression tasks, i.e., Mean square error (MSE), Pearson correlation coefficient ( $r$ ) and residual analysis method. Additionally, the model learning curves were evaluated which summarized the training process i.e., a plot of a train, and validation loss (MSE) over training epochs. Specifically, this plot provided insights into the training progress, such as the model convergence rate, overfitting or underfitting. Therefore, learning curves for each model were closely monitored. Furthermore, the

residual analysis was performed to assess the model quality and identify any systematic patterns between the predicted and actual values. First, a trained model was used to predict the target variable from the input feature. A predicted versus actual variable plot was established, and the correlation coefficient ( $r$ ) was computed, representing the strength and direction of the linear relationship. The model residuals were calculated by subtracting the predicted values from the actual. This computed difference was plotted and analyzed to check the residual distribution and detect patterns or outliers. The correlation coefficient and MSE measured the model accuracy and goodness of fit. If the model's performance was satisfactory, the models' weights were saved, for future prediction for each output variable. The training progress, i.e., train and validation loss (MSE) metrics, were saved and stored. If the model performance was not satisfactory, the ANN model was further refined iteratively by adjusting the hidden layer structure (size and depth), activation function, hyperparameters, and optimization algorithms. The size of neurons was limited to a maximum of 75 neurons, and the maximum layers (depth) were limited to 5. The sigmoid and ReLu activation functions were implemented in the hidden layer, keeping linear in the output layer. The optimization algorithms included Adam, Stochastic Gradient Descent (SGD), and Root Mean Square Propagation (RMSProp). The other hyperparameters, such as learning rate, varied from 0.0001 to 0.0006. The model parameter was optimized until the acceptable or best model performance was observed.

#### **7.2.4 ANN model interpretation**

ANN models are known for automated learning of complex input-output relationships from the available. However, it is often considered as a black box and does not provide a meaningful or explicit relationship between input and output feature unlike mathematical models or multiple regression models. However, it is essential for milling or baking operation managers to

understand which input feature is of high or least importance to output feature in order to make a meaningful decision on milling or baking operations. Therefore, a feature importance method was used to understand and measure each input feature's contribution toward the ANN prediction. Feature importance identified the most or least prominent features and their contribution to the predicted variables. Various methods are available to determine the feature importance, but we implemented the two most common methods used in regression tasks. The selected methods included permutation importance, and Shaply value. The feature importance was performed on the final best model for each output variable.

#### **7.2.4.1 Permutation importance**

Permutation importance is often used for feature selection, feature importance, and identifying data issues in a machine learning model. In permutation importance, each input feature is shuffled randomly while other features are kept unchanged to assess the importance of the shuffled feature. When a feature is shuffled, model performance change is recorded and quantified to determine its impact on model prediction. This study used a Python library called ELI5 (Explain Like I'm 5) to compute the feature importance and gain insight into ANN models. The following steps were performed using ELI5: (1) Train and evaluate model performance: The final best ANN model trained on a given dataset was used, and its baseline performance was evaluated before computing feature importance. (2) Calculate Feature Importance: The feature importance (weights) was calculated by shuffling the values of each feature and evaluating its impact on model performance compared to the baseline. (3) Result Interpretation: The calculated feature weights were ranked based on their scores. A significant drawback of feature importance is that it does not indicate whether a feature's contribution towards the model prediction is

positive or negative. On the other hand, the Shapley values can explain if the features had positive or negative contributions to model predictions.

#### **7.2.4.2 Shapley values**

Shapley values originated from cooperative game theory and are often used to gain insight into machine learning models. Shapley values help quantify the contribution of each feature within a prediction model towards the outcome. Shapley values provide a fair way to distribute the "credit" for a prediction among its individual features, considering all feature combinations and their respective contributions. It offers a comprehensive understanding of how distinctive features impact model predictions, making it a valuable tool for model interpretation and analysis. This study used a Python library called SHAP (SHapley Additive exPlanations) that provided a unified framework for explaining the trained ANN output. The SHAP library computed SHAP values, created a summary plot, and mathematical details can be found here (Lundberg & Lee, 2017) The Shapley values assigned the contribution of each feature to the prediction of an individual instance.

### **7.3 Results and Discussion**

#### **7.3.1 Flour properties**

The compositional and rheological properties of wheat flour samples are summarized in Figure 7.3. The sample protein content varied from 9.05 to 16.8%, aligning with the typical protein range of winter wheat cultivated in the region (Jaenisch et al., 2019; Lollato et al., 2019; Maeoka et al., 2020; Raj et al., 2023). Environmental (e.g., temperature, drought, and rainfall), and genetic factors along with management practices (e.g., fertilization and irrigation) can alter the wheat protein content and concentration (Jaenisch et al., 2022; Lollato et al., 2021; Tian et al., 2022; Wilson et al., 2020). Therefore, the dataset used in this study deliberately encompassed

different environments, winter wheat varieties with diverse milling and baking attributes, and management practices with the objective of increasing the variability in the measured attributes for modelling purposes. In this study, the FNV varied from 269 to 836 s and the ash content was 0.49% (Fig. 7.3). FNV analysis is a rapid method to assess  $\alpha$  – amylase activity of the grains and to predict bread baking quality. The enzyme ( $\alpha$  – amylase) hydrolyzes the starch in wheat flour impeding the formation of an essential starch – protein network affecting the dough structure. A higher  $\alpha$ - amylase activity leads to a lower FNV. Furthermore, low FNV indicates sprouting damage and poor baking quality. In general, FNV between 300 and 450 s or higher is associated with better baking quality and price premiums (He et al., 2019).

Ensuring high quality of baked products relies significantly on achieving optimal rheological properties. WA denoted the quantity of water absorbed by flour to attain an optimal dough consistency and is dependent upon factors like protein content, damaged starch, and other polysaccharides within the flour matrix (Ma et al., 2007). In the studied samples, WA was around 65% (Fig. 7. 3) which is considered optimal (Biel et al., 2021) for the bread dough. DDT and DS are intrinsically linked to protein content as flours with higher protein content tend to exhibit extended DDT and DS (Cui et al., 2023). Figure 4 illustrates the correlation between the measured flour properties and dough characteristics. In this study, there was a positive correlation between protein content and the rheological properties (WA, DDT, and DS). Additionally, FNV and ash have a positive influence on WA as reported by (Codină et al., 2019). Conversely, moisture content exhibited negative correlations with WA ( $r = -0.36$ ) and DDT ( $r = -0.11$ ).

### 7.3.2 ANN Model development and evaluation

A multi-layer perceptron type ANN was trained with back propagation algorithm to predict the rheological properties of dough as a function of flour properties i.e., moisture content (%), protein content (%), ash content (%) and falling number value (s). Independent ANN models were developed to predict each farinograph variable i.e., water absorption (WA), dough development time (DDT), and dough stability (DS). The hidden layer size (maximum 4) and neurons (5 to 75) were iteratively varied in increasing order while tracking the performance of each ANN architecture on wheat data. The ANN performance was influenced by the number of neurons in the hidden layer and the size of hidden layers, while early stopping was found effective to avoid overfitting. Table 7.1 presents the best performing ANN model for each output feature along with performance statistics. For WA and DDT, the best ANN model included two hidden layers while, the optimal configuration for DS included four hidden layers to capture the complex relationship from the data. The optimum number of neurons in hidden layers varied from 5 to 60 among these models. The learning rate was adjusted for model training and ranged between 0.0001 to 0.0003 for the best performing models.

The model performance was examined, and for each output variable, the ANN model with the lowest MSE and highest  $r$  was selected (Table 7.1). The  $r$  values for ANN- WA, ANN-DDT, and ANN-DS were 0.79, 0.79 and 0.63, respectively, on the model development set (train and validation). The  $r$  values of test set were varied from 0.46 to 0.74, this could be attributed towards having only 20 samples in test subset that resulted in poor  $r$  value. The training MSE was 0.34, 0.26 and 0.48 for WA, DDT, and DS, respectively.

The learning curves presented the model learning progress during training and Figure 7.5 depicted the learning curves for WA, DDT, and DS ANN models. The loss declined rapidly for

initial epoch (< 25 epochs) with subsequent gradual decline until the training was stopped. The implemented early stopping method stopped the ANN training at 380, 411 and 150 epochs for WA, DDT, and DS model, respectively. The early stopping was effective against overfitting (Badgujar et al., 2023), since the training was stopped when no improvement was observed in loss for 60 epochs (observed for WA & DDT, Fig. 7.5a & 7.4b) or loss started to increase after reaching the lowest degrading the model performance (observed for DS, Fig. 7.5c). Additionally, the loss reduced smoothly for WA and DS model than DDT which showed frequent pikes in validation loss, perhaps because of higher learning rate for DDT model ( $lr = 0.0003$ ). The learning curves analysis proved instrumental in gaining insights into the potential risk of overfitting within the constructed model.

Regression analysis was performed and Figures 7.6, 7.7 and 7.8 plot predicted versus actual values, and regression residuals for WA, DDT, and DS. The plot of predicted versus actual values showed scattered data points closely aligning with a unity slope for WA (Fig. 7.6a) and DDT (Fig. 7.7a) which suggested a reliable performance. Meanwhile, the data points were scattered unevenly especially at higher positive values for DS models (Fig. 7.8a) which suggest satisfactory performance. Furthermore, the residual plot (Fig. 7.6b, 7.7b and 7.8b) showed a random distribution of the residuals, without any definite pattern for the output variable (WA, DDT, and DS) indicating the goodness of fit of the developed ANN model. We acknowledge that the ANN models were developed using only 192 data samples and having more data could potentially improve model performance.

The trend of predicted and actual values was compared for developed ANN model (Fig. 7.9) to assess its accuracy and detecting patterns or outliers. The predicted values closely aligned and followed the actual values for WA and DDT with few outliers, indicating a strong predictive

performance (Fig. 7.9a, b). However, the actual values of DS were less stable, showing frequent and multiple peaks (Fig. 7.9c) challenging the development of ANN models to capture this variability, even when using the more complex ANN model architecture (4-30-60-10-5-1) and resulted with satisfactory ANN model performance ( $r = 0.63$ ). This is because the variables selected for the study, especially grain protein content, may not have been able to capture all the variations in stability. Grain protein content, the major determinant of dough rheology, is comprised of complex proteins such as gliadins, glutenins, asperagine, glutamine, arginine, and proline (Žilić et al., 2011). The compositions of these proteins, especially glutenins and gliadins, can influence dough rheology (Xue et al., 2019). For instance, the differences in proportion of glutenin and subsequent variation in the gliadin – glutenin ratio can significantly influence the DDT and DS (Dhaka & Khatkar, 2015). The quality and proportion of these proteins are dependent on genetic factors (genotype), environmental factors, management factors and their interactions (Marchetti et al., 2012). The inclusion of NIR measurements encompassing protein components such as gliadin and glutenin has the potential to enhance the applicability of the model to various types of wheat flour and further improve its predictability (Abbasi et al., 2014).

### **7.3.3 ANN model interpretation**

The permutation importance computed the weights of each feature for prediction and ranked each input variable as shown in Figure 7.10. A higher score indicates a more important feature, meaning that the model heavily relies on it for making accurate predictions. In other words, these rankings provide insights on features that are most influential in the model's decision-making process. The weights of input parameters vary in the order of protein, ash, falling number and moisture content for WA and DS (Fig. 7.10b &f). This was analogous with the correlation plot (Fig. 7.4). Variable contribution analysis indicated that model relies on the protein content for

estimation of the properties: WA, DDT, and DS. This permutation importance and Shapley value methods opened the black box ANN model by providing an insight into how model predictions are made and which features are most influential. The influence of protein on the dough characteristics like WA, DDT and DS was also outlined in the studies of (Dowell et al., 2006; Saint Pierre et al., 2008). In hard winter wheats, the increase in protein content is associated with increase in monomeric protein (gliadin) which in turn modifies the rheological properties (Saint Pierre et al., 2008; Sapirstein et al., 2018).

SHAP analysis explains the significance of the features on the model and provides visualizations of feature contributions (Rodríguez-Perez & Bajorath, 2020a). Consequently, Shapley values serve as assessments of both the significance (quantitative value of the contribution) and the orientation (direction) of feature importance (Rodríguez-Perez & Bajorath, 2020b). For instance, protein content (feature) with positive sign contributes to WA prediction whereas, moisture content with negative sign has negative contribution in the prediction model (Fig. 7.10 b). Thus, feature importance illustrates the variable contributions and enables interpretation of the NN model. Moreover, it transforms the “black box” nature of the approach to an interpretable output.

The study found that ANN models can be used to capture the non-linear interaction between wheat dough rheological properties as a function of flour properties. The major learning on data processing, model development, and validation can be easily applied to other wheat varieties and flour properties to gain more insight into understanding and exploring the existing relationship, which was not previously possible with either empirical or mathematical models.

## 7.4 Conclusions

Wheat flour being a major ingredient in numerous foods products, its physical, chemical, and rheological properties determine the economic value and characteristic of the final product (Mutlu et al., 2011). In this study, we explored the ability of ANN to predict the rheological characteristics of wheat dough in terms of NIR measurements (protein content, moisture content, ash content) and falling number value. Feed forward multilayer perceptron models were developed for each output variable: WA, DDT, and DS. The number of hidden layers in the best fitting models, characterized by lowest MSE and highest  $r$  values, ranged from two to four, with each layer containing 5 to 60 neurons. Early stopping method employed in the study prevented overfitting of the model. Moreover, permutation importance and shapley value method investigated the black box ANN model and provided an insight on how the model makes predictions and which features are most important. Shapley value asserts the significance of protein content in network predictions.

The ANN model proved to be a valuable tool for predicting the functionality of wheat flour, particularly with respect to parameters such as WA, DDT, and DS. In comparison to conventional methods used to determine farinograph parameters, the developed model is rapid and simple. However, it is essential to acknowledge a potential limitation of the model, which is its reliance on a limited data set primarily comprised of hard winter wheat varieties. To address this limitation and advance the research our future endeavors will focus on expanding the scope of our model to encompass various wheat classes including spring wheat. This expansion, by incorporating more diverse datasets, will lead to further refinement and enhancement of the predictive model.

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## Tables

**Table 7.1. Summary of best performing ANN model for each output feature**

| Output | ANN<br>architecture | Learning<br>rate | MSE      |            |      | r (correlation coefficient) |          |
|--------|---------------------|------------------|----------|------------|------|-----------------------------|----------|
|        |                     |                  | Training | Validation | Test | r (train+<br>Val)           | r (test) |
| WA     | 4-20-10-1           | 0.0002           | 0.34     | 0.46       | 1.20 | 0.79                        | 0.46     |
| DDT    | 4-30-10-1           | 0.0003           | 0.26     | 0.64       | 0.92 | 0.79                        | 0.74     |
| DS     | 4-30-60-10-5-1      | 0.0001           | 0.48     | 0.67       | 0.74 | 0.63                        | 0.68     |

## Figures

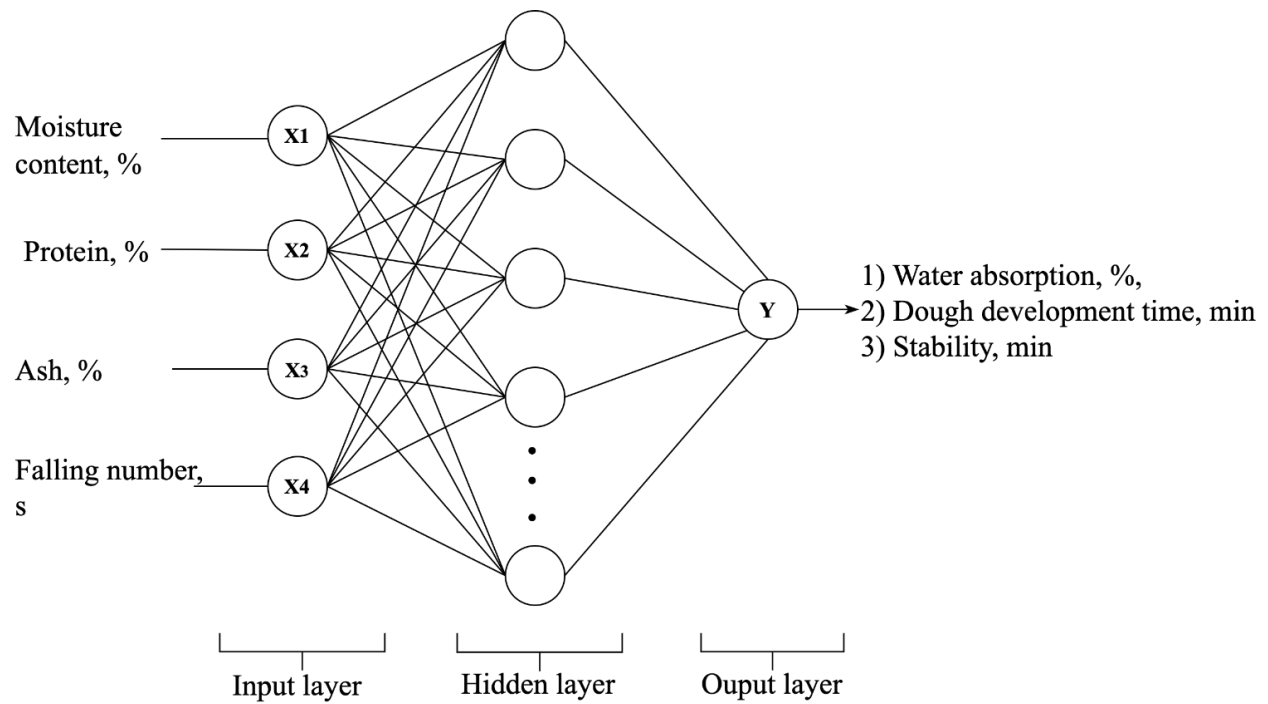


**Figure 7.1. Implemented multi-layered, feedforward ANN architecture with selected input and output features**

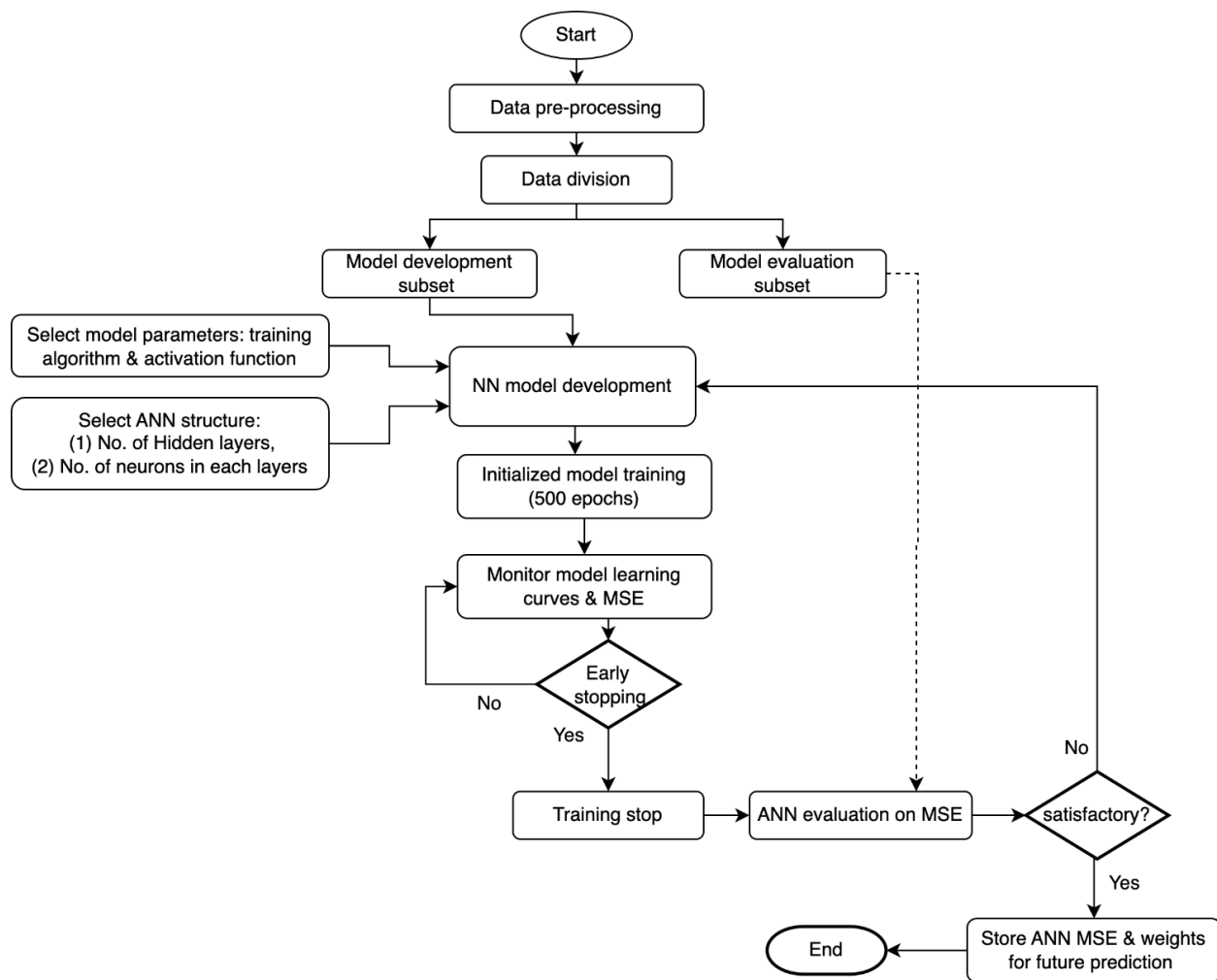


**Figure 7.2. Implemented ANN model development and training process for predicting the rheological properties of wheat dough**

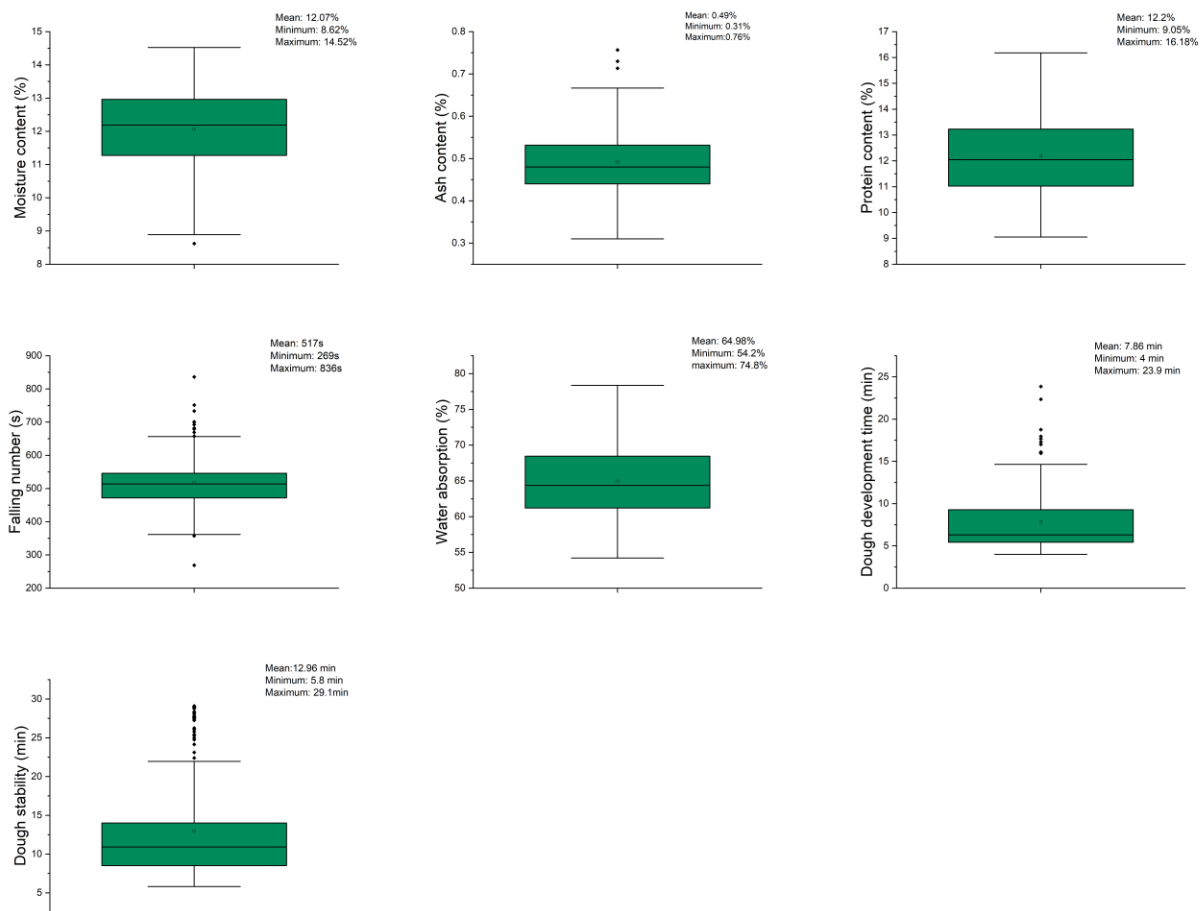


**Figure 7.3. Box plot of the experimental data based on ANN modelling (192 samples) ( ■ 25%~75%; ○ Median; — Mean; ◇ Outliers)**

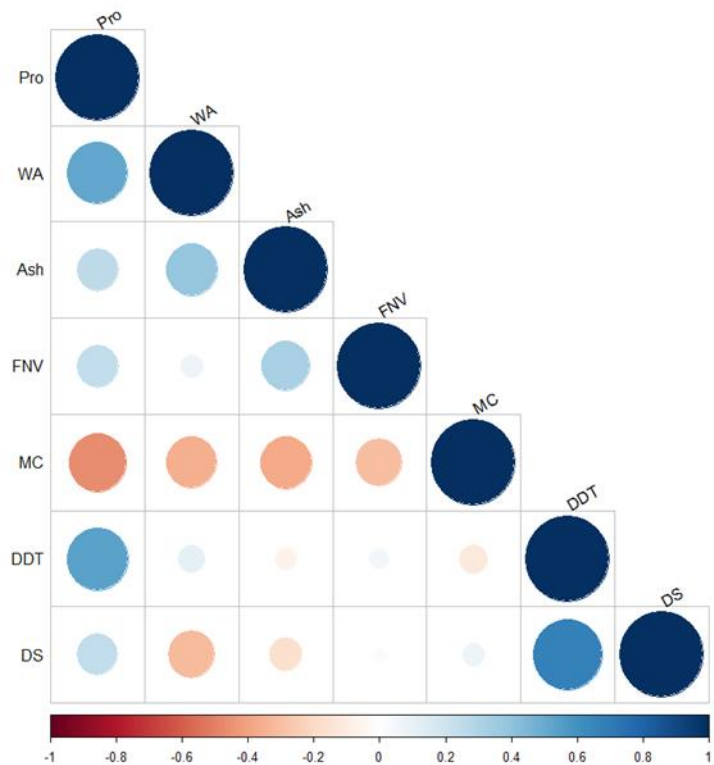


**Figure 7.4. Correlation matrix of flour properties and rheological characteristics at 95% confidence level. (Pro: protein content, FNV: Falling number value, MC: moisture content, WA: water absorption, DDT: dough development time, DS: dough stability)**

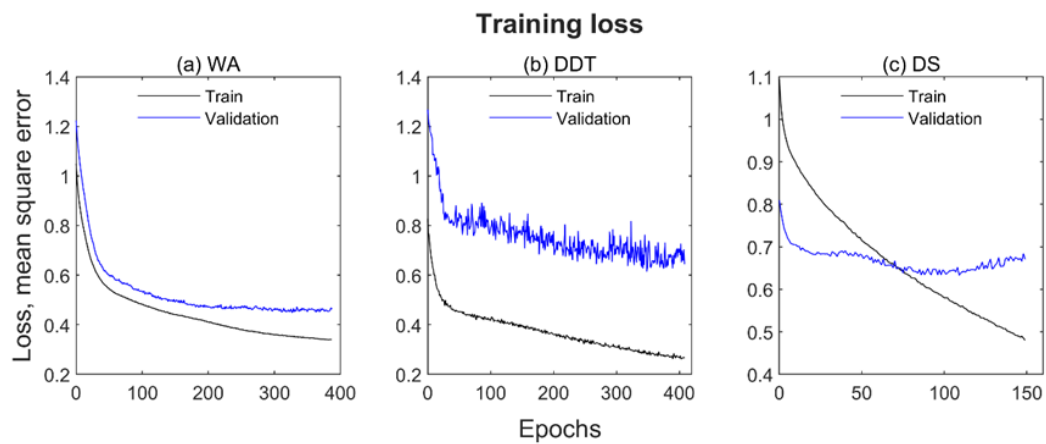


**Figure 7.5. Learning curves for selected ANN models: (a) water absorption (WA), (b) dough development time (DDT), (c) dough stability (DS)**

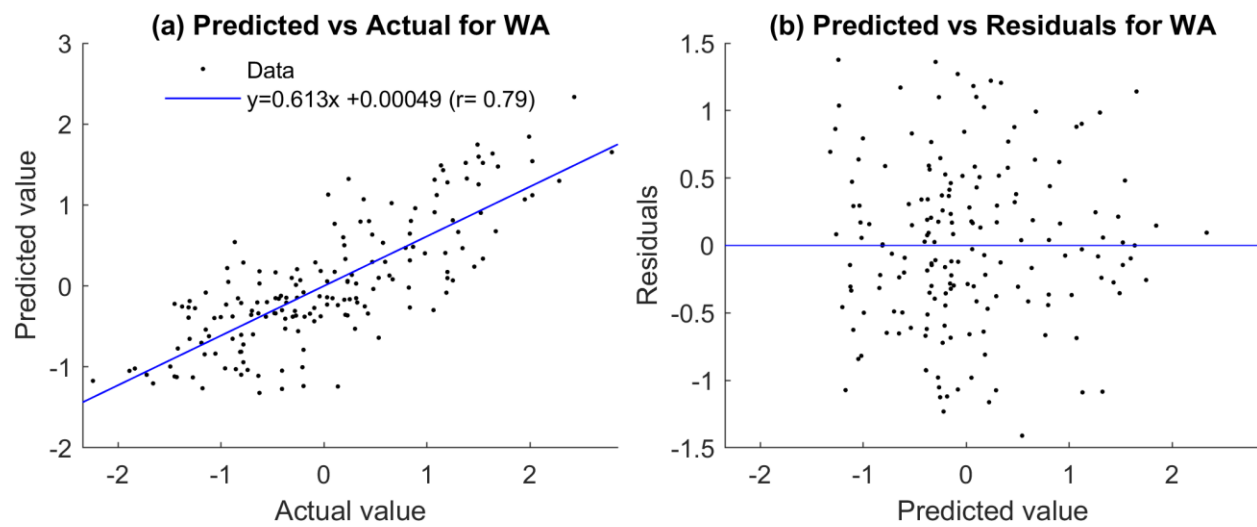


**Figure 7.6. Regression analysis for water absorption (WA): (a) predicted vs actual values  
(b) predicted vs residual**

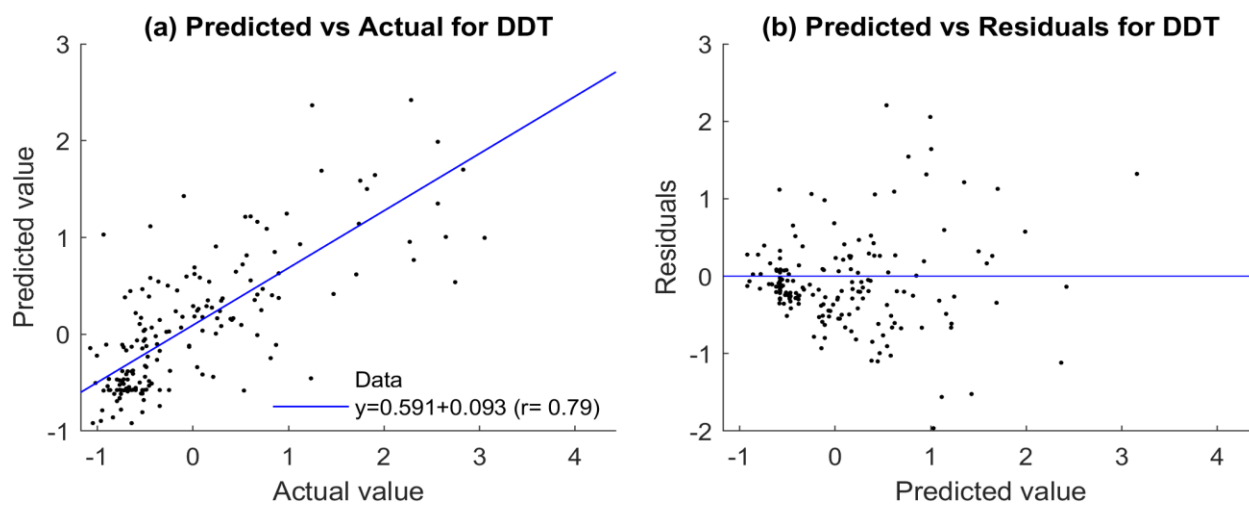


**Figure 7.7. Regression analysis for dough development time (DDT): (a) predicted vs actual values (b) predicted vs residual**

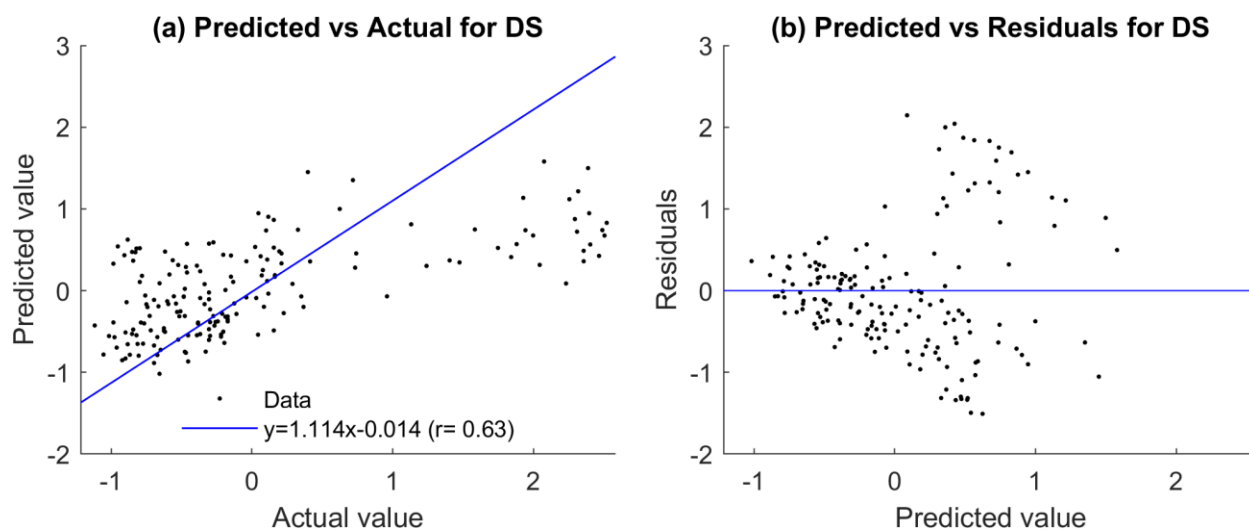


**Figure 7.8. Regression analysis for dough stability (DS): (a) predicted vs actual values (b) predicted vs residual**

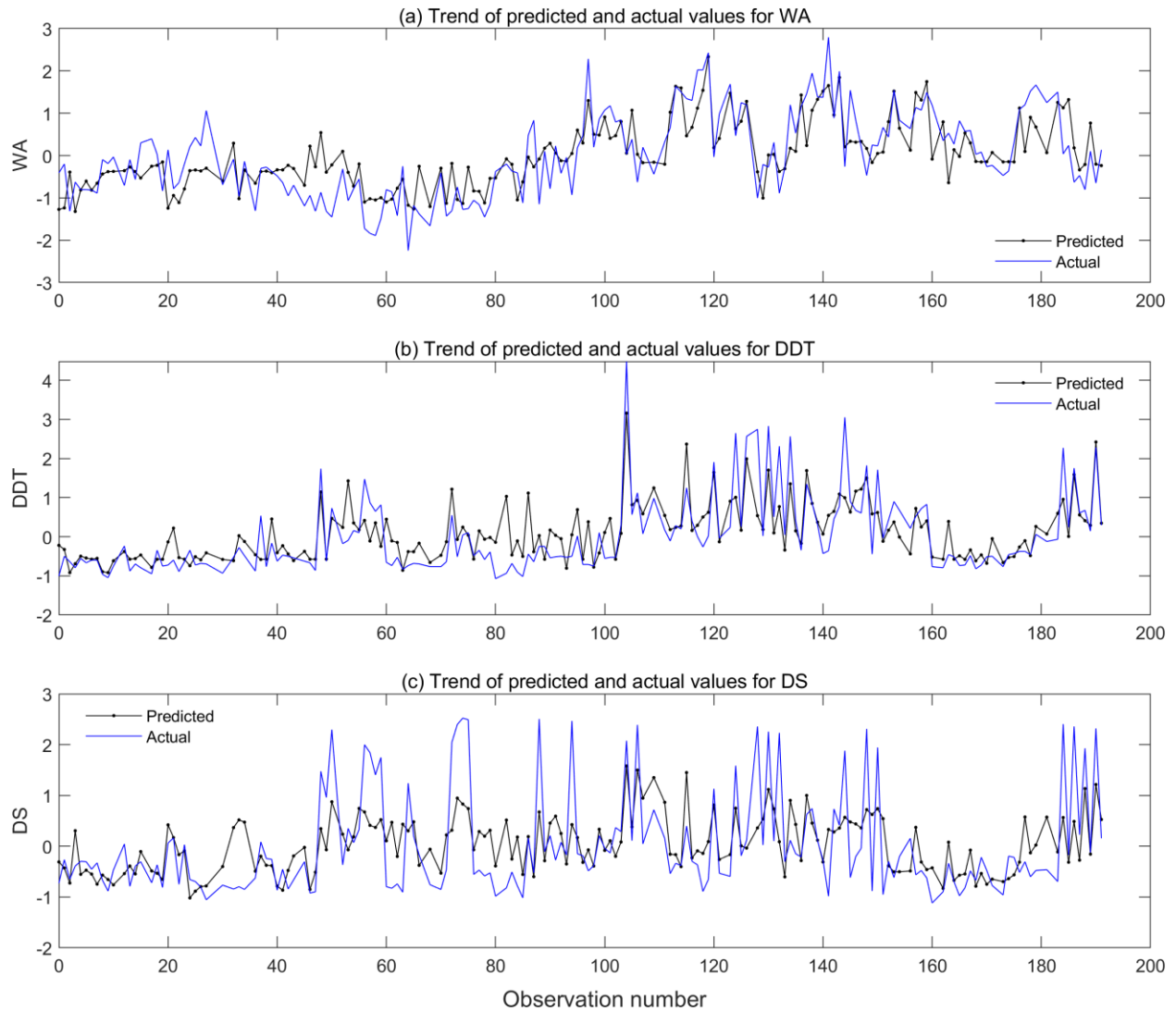


**Figure 7.9. Trend of predicted and actual observation for selected best ANN model: (a) Water absorption (WA), (b) Dough development time (DDT), and (c) Dough stability (DS)**

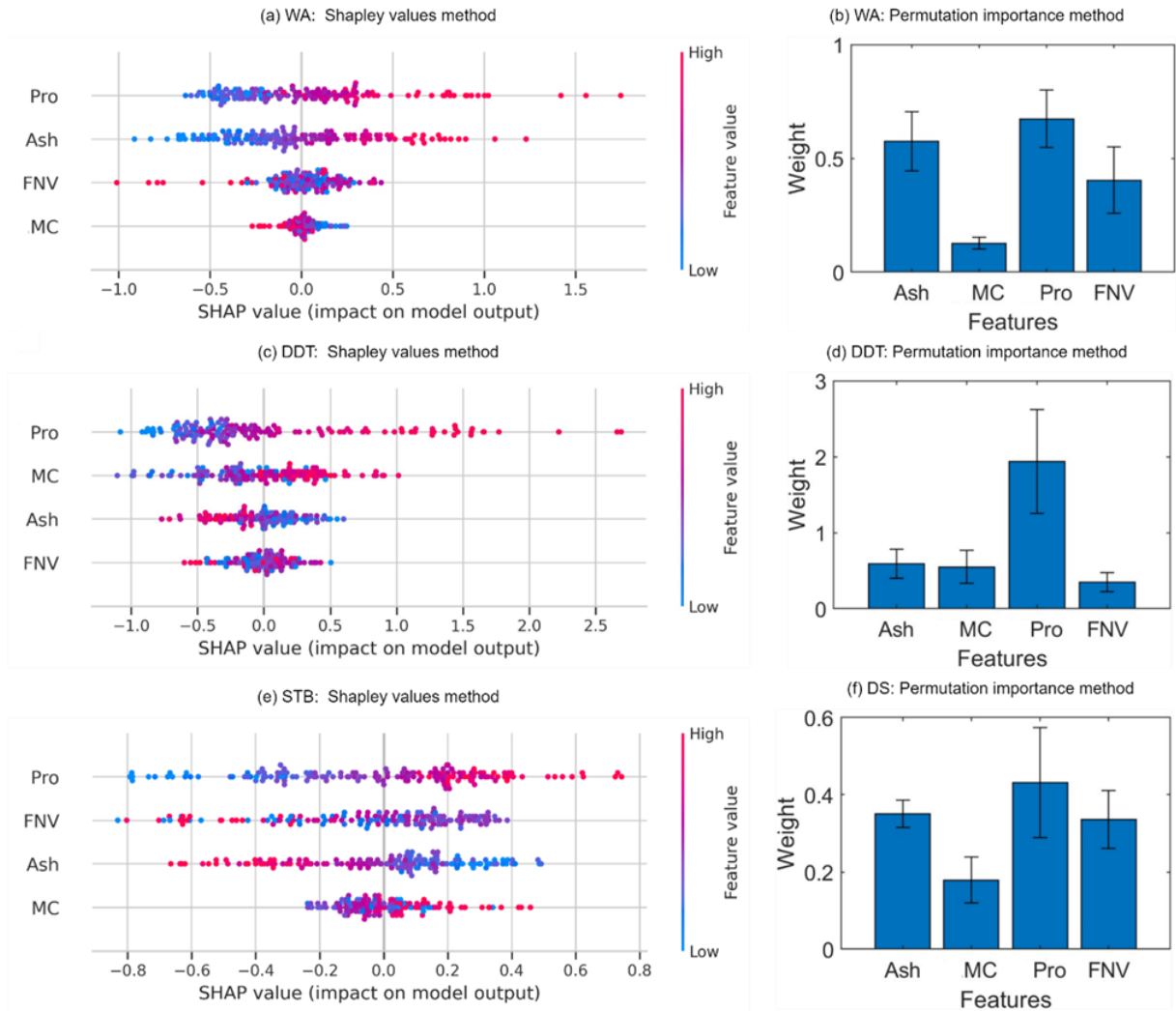


**Figure 7.10. ANN model interpretation with permutation importance and shapley value for Water absorption (WA), Dough development time (DDT), and Dough stability (DS)**

## Chapter 8 Conclusion and Future Scope

Wheat bread, a staple food for millions, is made from flour, water, leavening agent, and salt. Its baking quality depends on various factors, including grain variety, growing conditions, and milling. This study investigated the effects of preharvest interventions and post-harvest processing on the baking quality of hard wheat, which is primarily used for production of leavened bread. Specifically, the research focused on (i) concurrently increasing the wheat yield and baking quality through crop management practices, (ii) understanding the mechanistic aspects of tempering and its impact on the wheat kernel behavior, and (iii) investigating the role of blending in flour functionality. The following paragraphs brief on the conclusions drawn from the study.

Management practices (pre-harvest intervention including foliar fungicide application and nitrogen fertilization) can concurrently increase the yield and improve the rheological properties of the dough and baking quality.

- High input management practices (foliar fungicide application + nitrogen fertilization), [i.e., up to 134 kg N ha<sup>-1</sup> (applied as urea) than normal farmer practices, 22 kg S ha<sup>-1</sup> (applied as gypsum), 45 kg Cl ha<sup>-1</sup> and 50 kg K ha<sup>-1</sup> (applied as KCl), two fungicide applications] increased yield (4206 kg ha<sup>-1</sup>) and simultaneously improved milling and baking quality.
- High input – N (i.e., foliar fungicide application), [i.e., N rate was applied as urea (460 g N kg<sup>-1</sup>) to match a yield goal of ~4,000 kg ha<sup>-1</sup>, 22 kg S ha<sup>-1</sup> (applied as gypsum), 45 kg Cl ha<sup>-1</sup> and 50 kg K ha<sup>-1</sup> (applied as KCl), two fungicide applications] improved milling

attributes such as thousand kernel weight, test weight, flour yield and reduced the flour ash.

- High input – fungicide (i.e., nitrogen fertilization), [i.e., up to 134 kg N ha<sup>-1</sup> (applied as urea) than normal farmer practices, 22 kg S ha<sup>-1</sup> (applied as gypsum), 45 kg Cl ha<sup>-1</sup> and 50 kg K ha<sup>-1</sup> (applied as KCl)] increases in water absorption, dough stability and loaf volume.

Tempering of the wheat kernels can impart changes in the milling quality and baking properties of the wheat. Thus, it is important to understand the moisture distribution inside the kernels as well as the influence of time on the process.

- A finite element model was developed to analyze moisture distribution within single wheat kernels.
- The core of the kernel reached tempering moisture levels in 12h, contrary to the conventional 24h, considering the kernel as a homogeneous entity.
- Magnetic resonance imaging (MRI) analysis validated the moisture distribution by the FEM model.
- Studying the change in mechanical properties of the kernel during the tempering process, revealed that tempering time can significantly impact compressibility.
- Hard red winter (HRW) and hard red spring (HRS) samples exhibit similar yet distinct changes in the compressibility and viscoelastic properties during tempering.
- The kernel compressibility during tempering follows first order kinetics. The compressibility rate ranged from 0.002 to 0.0057 h<sup>-1</sup> for HRS and from 0.0026 to 0.0066 h<sup>-1</sup> for HRW, respectively.

These findings provide valuable insights in the optimization of the tempering process with respect to the wheat class by reducing time, ultimately improving overall efficiency.

Further, the impact of the tempering conditions (moisture and time) on the chemical and rheological properties of flour from blends of hard red wheats were analyzed.

- Blending the HRW and HRS significantly influenced the particle size, damaged starch content and protein content, subsequently modifying the rheological properties.
- Increased proportion of HRS in the blend decreased the pasting temperature range (from 18.39 °C for B1 to 14.21 °C for B3) of the dough.
- Variations in the properties were also exhibited by successive milling streams. Protein content varied notably among break flour streams (13.41% in 1 BK to 16.75% in 3 BK), while damaged starch content varied in the reduction streams across all blends (10.13% in 1M to 15.58% in 3M).

Further, an artificial neural network (ANN) model was developed to predict the rheological characteristics of the wheat dough in terms of NIR measurements (protein content, moisture content, ash content) and falling number value.

- Feed forward multilayer perceptron models were developed for each output variable: WA, DDT, and DS.
- The number of hidden layers in the best fitting models, ranged from two to four, with each layer containing 5 to 60 neurons.
- Feature importance analysis (Shapley value) highlighted the significance of protein content in network predictions.

This study demonstrates the potential of data-driven ANN models in predicting the rheological characteristics of dough. In comparison to conventional methods used to determine farinograph parameters, the developed model is rapid and simple.

Thus, the comprehensive investigation provides valuable insights into various aspects of hard winter wheat production and processing, aiming to enhance both yield and quality attributes. Furthermore, these findings offer valuable insights into the interplay between tempering conditions and kernel properties, facilitating the optimization of tempering processes for enhanced efficiency. The analysis of flour blends and development of predictive models for dough rheological properties further contribute to our understanding of wheat processing and its impact on product quality. These results and the developed models could serve as a decision support tool and aid millers in adjusting the mill settings and bakers in modifying the dough mixing based on dough rheology.

## **Future Scope**

The initial phase of the study successfully demonstrated simultaneous improvement of yield and quality, albeit limited to a small set of locally adapted genotypes within the same commercial class. To broaden the conclusions, future studies should incorporate a wider range of genotypes and assess the potential long-term effects of increased nitrogen application on soil health and environmental sustainability. Additionally, the simplification of considering the wheat as a homogeneous entity in the FEM overlooks the heterogeneous diffusion characteristics of its components, such as endosperm, pericarp, and germ. Future models should aim to incorporate these complexities for more accurate predictions. Furthermore, exploring three-dimensional analysis of the moisture migration with porous modelling could provide deeper insights. Moreover, there is a potential for further exploration of blending to develop clean label products.

While the ANN model shows promising predictability, it is essential to acknowledge its reliance on a limited data set primarily comprised of hard winter wheat varieties, which poses a potential limitation. To address this limitation and advance the research our future endeavors will focus on expanding the scope of our model to encompass various wheat classes including spring wheat. This expansion, by incorporating more diverse datasets, will lead to further refinement and enhancement of the predictive model.

## Appendix A

**Supplemental Table S1.** *Parentage of the genotypes included in the current study.*

| Genotype      | Parentage                         |
|---------------|-----------------------------------|
| WB4269        | KS98W0512-2-4/HV9W02-846R//Armour |
| WB4303        | KS940786-7//G982163/G982002       |
| WB4458        | KS940786-7//G982163/G982002       |
| WB4515        | KS980259-4-5//NUHILLS/HV9W00-993W |
| WB-Grainfield | G982231/G982159//KS920709W        |

**Supplemental Table S2.** *Dates of major management activities in the trials conducted in Manhattan (MAN), Hutchinson (HUT), Belleville (BEL), and Ashland Bottoms (ASB), Kansas, during the growing seasons of 2016-17 (17), 2017-18 (18), and 2018-19 (19)*

| Environment | Planting date | N fertilization<br>(Feekes 4) | Early fungicide date<br>(Feekes 6) | Late fungicide date<br>(Feekes 10.5) | Harvest   |
|-------------|---------------|-------------------------------|------------------------------------|--------------------------------------|-----------|
| MAN17       | 11/17/2016    | 3/22/2017                     | 4/7/2017                           | 5/2/2017                             | 6/17/2017 |
| HUT17       | 10/13/2016    | 2/17/2017                     | 4/3/2017                           | 4/26/2017                            | 6/19/2017 |
| BEL18       | 10/19/2017    | 3/8/2018                      | 4/27/2018                          | 5/17/2018                            | 6/27/2018 |
| HUT19       | 10/22/2018    | 3/18/2019                     | 4/16/2019                          | 5/15/2019                            | 6/26/2019 |
| MAN19       | 10/23/2018    | 3/22/2019                     | 4/24/2019                          | 5/20/2019                            | 7/1/2019  |
| ASB19       | 11/1/2018     | 3/22/2019                     | 5/2/2019                           | 5/31/2019                            | 7/1/2019  |

**Supplemental Table S3.** Initial soil fertility information at sowing at Manhattan (MAN), Hutchinson (HUT), Belleville (BEL), and Ashland Bottoms (ASB), Kansas, during the growing seasons of 2016-17 (17), 2017-18 (18), and 2018-19 (19). Soil test includes soil pH, Mehlich-3 extractable phosphorus (P), potassium (K), calcium (Ca), magnesium (Mg), sodium (Na), ammonium nitrogen (NH<sub>4</sub>-N), nitrate nitrogen (NO<sub>3</sub>-N), and organic matter (OM). Sampling depths were 0 to 15 cm and 15 to 45 cm in 2016-17 and 0 to 15 cm and 15 to 60 cm in 2017-18. Source: (Jaenisch et al., 2019)

| Environment | Depth   | OM  | pH  | NO3-N               | P  | K   | Ca   | Mg  | Na    | SO4-S | Cl   | CEC                     | Sand | Silt | Clay |
|-------------|---------|-----|-----|---------------------|----|-----|------|-----|-------|-------|------|-------------------------|------|------|------|
|             | cm      | %   |     | kg ha <sup>-1</sup> |    |     |      |     | ppm   |       |      | meq 100 g <sup>-1</sup> |      | %    |      |
| MAN17       | 0 – 15  | 4.0 | 7.5 | 19                  | 29 | 269 | 4246 | 220 | 12.3  | 8.8   | 6.9  | 23.8                    | 14   | 54   | 32   |
| MAN17       | 15 – 60 | 3.3 | 7.9 | 61                  | 26 | 292 | 5610 | 281 | 16.8  | 5.3   | 4.1  | 31.2                    | 18   | 46   | 36   |
| HUT17       | 0 – 15  | 2.6 | 7.5 | 14                  | 58 | 318 | 3851 | 172 | 15.3  | 5.4   | 3.3  | 21.6                    | 32   | 42   | 26   |
| HUT17       | 15 – 60 | 2.7 | 8.0 | 37                  | 38 | 288 | 4725 | 173 | 16.5  | 5.0   | 3.4  | 25.9                    | 30   | 38   | 32   |
| BEL18       | 0 – 15  | 2.8 | 5.4 | 11                  | 50 | 509 | 2091 | 419 | 21.5  | 4.1   | 4.7  | 28.7                    | 10   | 60   | 30   |
| BEL18       | 15 – 60 | 2.4 | 5.8 | 28                  | 22 | 426 | 3392 | 698 | 65.7  | 4.1   | 4.9  | 32.1                    | 8    | 50   | 42   |
| HUT19       | 0 – 15  | 1.9 | 6.3 | 44                  | 55 | 160 | 1704 | 229 | 73.0  | 9.5   | 9.4  | 17.6                    | 44   | 36   | 20   |
| HUT19       | 15 – 60 | 1.7 | 7.6 | 82                  | 8  | 164 | 4042 | 437 | 244.0 | 23.4  | 13.2 | 25.3                    | 42   | 30   | 28   |
| MAN19       | 0 – 15  | 3.5 | 6.2 | 6                   | 22 | 162 | 2977 | 357 | 17.0  | 2.5   | 7.5  | 26.3                    | 16   | 58   | 26   |
| MAN19       | 15 – 60 | 2.8 | 7.0 | 16                  | 9  | 217 | 4477 | 411 | 26.0  | 3.5   | 9.1  | 26.5                    | 14   | 56   | 30   |
| ASB19       | 0 – 15  | 3.0 | 6.5 | 6                   | 8  | 304 | 3329 | 550 | 21.0  | 2.6   | 8.2  | 22.1                    | 12   | 50   | 38   |
| ASB19       | 15 – 60 | 2.2 | 6.7 | 10                  | 4  | 309 | 3604 | 760 | 36.0  | 2.2   | 6.6  | 25.3                    | 6    | 50   | 44   |

**Supplemental Table S4.** *Effect of tempering moisture on particle characteristics and chemical properties of straight grade flours of wheat blends*

| Tempering moisture (%) | Sample | Flour yield (%) | d10 (μm)    | d50 (μm)     | d90 (μm)      | Protein (%) | Damaged starch (%) | Ash (%)     |
|------------------------|--------|-----------------|-------------|--------------|---------------|-------------|--------------------|-------------|
| 14                     | HRW    | 69.4 (4.0)      | 22.93 (1.1) | 75.57 (14.7) | 139.36 (13.4) | 9.72 (0.3)  | 7.98 (1.1)         | 0.53 (0.10) |
|                        | B1     | 75.5 (1.3)      | 24.69 (2.6) | 79.26 (11.6) | 127.18 (12.0) | 10.74 (0.6) | 9.07 (1.4)         | 0.51 (0.07) |
|                        | B2     | 72.6 (1.6)      | 22.55 (1.7) | 69.45 (6.0)  | 135.95 (18.1) | 12.81 (0.4) | 8.07 (2.8)         | 0.54 (0.05) |
|                        | B3     | 73.2 (0.7)      | 25.88 (2.7) | 76.09 (6.8)  | 124.17 (4.9)  | 13.31 (1.4) | 9.09 (1.8)         | 0.48 (0.08) |
|                        | HRS    | 67.9 (4.2)      | 28.15 (3.1) | 83.82 (4.9)  | 146.53 (1.8)  | 16.14 (1.3) | 9.90 (2.6)         | 0.50 (0.16) |
| 16                     | HRW    | 76.9 (4.0)      | 22.30 (1.1) | 61.17 (4.6)  | 127.60 (3.9)  | 9.11 (0.5)  | 8.10 (0.9)         | 0.49 (0.11) |
|                        | B1     | 73.6 (2.2)      | 23.95 (2.1) | 79.82 (9.4)  | 129.45 (3.1)  | 10.89 (0.3) | 8.42 (1.1)         | 0.47 (0.09) |
|                        | B2     | 72.8 (2.3)      | 25.26 (0.7) | 81.04 (6.8)  | 151.17 (13.6) | 11.40 (0.7) | 9.86 (1.8)         | 0.45 (0.03) |
|                        | B3     | 73.3 (3.4)      | 23.40 (0.4) | 81.95 (5.9)  | 132.17 (5.0)  | 13.34 (1.8) | 8.79 (3.0)         | 0.56 (0.23) |
|                        | HRS    | 72.7 (2.8)      | 24.82 (2.3) | 83.68 (13.1) | 150.57 (7.8)  | 15.68 (0.3) | 10.32 (2.8)        | 0.54 (0.11) |
| 18                     | HRW    | 74.0 (6.1)      | 22.62 (1.0) | 70.34 (3.2)  | 128.49 (4.0)  | 9.40 (0.3)  | 8.89 (1.7)         | 0.53 (0.20) |
|                        | B1     | 73.9 (5.0)      | 21.66 (2.6) | 63.62 (5.5)  | 133.80 (8.8)  | 9.68 (0.9)  | 9.64 (1.6)         | 0.46 (0.12) |
|                        | B2     | 74.4 (4.2)      | 24.46 (1.9) | 74.76 (4.5)  | 135.90 (3.8)  | 11.42 (0.6) | 10.11 (1.5)        | 0.51 (0.17) |
|                        | B3     | 72.2 (1.3)      | 22.74 (2.4) | 75.24 (7.2)  | 133.65 (10.6) | 12.17 (1.3) | 9.37 (2.1)         | 0.49 (0.04) |
|                        | HRS    | 71.2 (2.0)      | 23.35 (1.7) | 71.13 (6.1)  | 131.97 (7.0)  | 15.82 (0.3) | 9.46 (3.7)         | 0.59 (0.08) |

The values are represented as mean (± standard deviation). HRW: Hard red winter, HRS: Hard red spring, B1: Blend 1 (75% HRW: 25% HRS), B2: Blend 2 (50% HRW: 50% HRS), B3: Blend 3 (25% HRW: 75% HRS)

**Supplemental Table S5.** *Effect of tempering time on particle characteristics and chemical properties of straight grade flours of wheat blends*

| Tempering time (h) | Flour Yield |            | <i>d</i> 10       | <i>d</i> 50       | <i>d</i> 90       | Protein     | Damaged starch | Ash         |
|--------------------|-------------|------------|-------------------|-------------------|-------------------|-------------|----------------|-------------|
|                    | Sample      | (%)        | ( $\mu\text{m}$ ) | ( $\mu\text{m}$ ) | ( $\mu\text{m}$ ) | (%)         | (%)            | (%)         |
| 16                 | HRW         | 75.4 (3.5) | 21.96 (0.8)       | 66.38 (8.7)       | 132.87 (13.3)     | 9.45 (0.4)  | 9.05 (0.7)     | 0.48 (0.14) |
|                    | B1          | 74.5 (3.1) | 23.66 (2.3)       | 79.18 (12.1)      | 120.47 (7.9)      | 10.22 (0.9) | 8.35 (2.0)     | 0.50 (0.09) |
|                    | B2          | 75.5 (3.1) | 23.51 (2.4)       | 77.70 (4.5)       | 141.82 (13.1)     | 11.52 (0.8) | 10.37 (1.6)    | 0.39 (0.03) |
|                    | B3          | 71.9 (0.9) | 23.10 (0.5)       | 77.52 (7.1)       | 131.55 (12.3)     | 14.33 (0.8) | 10.35 (1.4)    | 0.45 (0.1)  |
|                    | HRS         | 71.4 (2.4) | 24.38 (1.1)       | 75.22 (3.1)       | 144.27 (6.1)      | 16.22 (1.2) | 9.07 (2.5)     | 0.52 (0.14) |
| 20                 | HRW         | 76.4 (3.0) | 22.96 (0.7)       | 65.96 (6.2)       | 117.61 (8.0)      | 9.30 (0.4)  | 8.61 (0.5)     | 0.56 (0.06) |
|                    | B1          | 75.7 (1.5) | 22.57 (4.3)       | 68.73 (7.0)       | 143.23 (13.4)     | 10.30 (0.3) | 8.64 (1.0)     | 0.46 (0.11) |
|                    | B2          | 73.6 (1.4) | 24.37 (2.3)       | 71.63 (8.1)       | 137.48 (15.4)     | 11.72 (0.8) | 9.82 (0.5)     | 0.50 (0.06) |
|                    | B3          | 74.5 (2.3) | 24.59 (1.0)       | 76.77 (3.8)       | 128.47 (5.1)      | 12.63 (2.2) | 10.09 (1.5)    | 0.57 (0.21) |
|                    | HRS         | 71.6 (1.1) | 26.31 (2.3)       | 80.86 (6.7)       | 141.18 (7.0)      | 15.92 (0.3) | 9.29 (1.7)     | 0.55 (0.1)  |
| 24                 | HRW         | 68.5 (4.0) | 22.93 (1.3)       | 74.75 (4.9)       | 144.98 (4.6)      | 9.47 (0.6)  | 10.09 (2.1)    | 0.61 (0.16) |
|                    | B1          | 72.8 (4.1) | 24.06 (1.0)       | 74.81 (4.0)       | 126.73 (4.9)      | 9.78 (1.3)  | 9.14 (2.0)     | 0.47 (0.09) |
|                    | B2          | 70.7 (0.4) | 24.40 (1.0)       | 75.93 (9.4)       | 143.72 (8.0)      | 11.84 (1.2) | 8.61 (3.0)     | 0.56 (0.12) |
|                    | B3          | 72.3 (1.6) | 24.32 (4.2)       | 78.99 (10.3)      | 129.97 (7.3)      | 13.85 (0.9) | 6.81 (0.8)     | 0.52 (0.07) |
|                    | HRS         | 68.8 (5.2) | 25.63 (5.2)       | 82.56 (7.1)       | 143.62 (7.5)      | 15.49 (0.3) | 9.52 (2.9)     | 0.55 (0.14) |

The values are represented as mean ( $\pm$  standard deviation). HRW: Hard red winter, HRS: Hard red spring, B1: Blend 1 (75% HRW: 25% HRS), B2: Blend 2 (50% HRW: 50% HRS), B3: Blend 3 (25% HRW: 75% HRS)

**Supplemental Table S6.** *Variation in particle characteristics and chemical properties of flour obtained from different milling streams (fraction)*

| Milling fraction | <i>d</i> 10       | <i>d</i> 50       | <i>d</i> 90       | Protein     | Damaged starch | Ash        |
|------------------|-------------------|-------------------|-------------------|-------------|----------------|------------|
|                  | ( $\mu\text{m}$ ) | ( $\mu\text{m}$ ) | ( $\mu\text{m}$ ) | (%)         | (%)            | (%)        |
| 1BK              | 40.78 (7.7)       | 96.89 (10.6)      | 167.19 (13.1)     | 13.47 (2.3) | 4.99 (1.3)     | 0.45 (0.2) |
| 2BK              | 39.02 (6.2)       | 74.61 (8.7)       | 144.56 (8.9)      | 15.01 (3.0) | 5.44 (1.4)     | 0.45(0.2)  |
| 3BK              | 31.76 (4.6)       | 79.89 (6.2)       | 128.97 (9.4)      | 16.89 (3.3) | 6.05 (1.6)     | 0.64 (0.2) |
| 1M               | 24.78 (3.7)       | 74.61 (11.2)      | 134.10 (8.4)      | 11.73 (2.4) | 8.82 (2.0)     | 0.47 (0.2) |
| 2M               | 22.45 (3.2)       | 69.05 (6.2)       | 128.11 (5.8)      | 11.31 (2.5) | 12.26 (2.7)    | 0.71 (0.2) |
| 3M               | 20.00 (2.0)       | 60.05 (13.7)      | 122.2 (8.8)       | 12.58 (2.2) | 14.92 (2.6)    | 1.17 (0.2) |

The values are represented as mean ( $\pm$  standard deviation). 1BK: 1<sup>st</sup> break roll, 2BK: 2<sup>nd</sup> break roll, 3BK: 3<sup>rd</sup> break roll, 1M: 1<sup>st</sup> reduction roll, 2M: 2<sup>nd</sup> reduction roll, 3M: 3<sup>rd</sup> reduction roll.